Calculating phase diagrams involving solid solutions via non-linear equations, with examples using THERMOCALC

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This is the starting point for the web-based material associated with the 1998 "Calculating phase diagrams" paper in Journal of Metamorphic Geology. It is all concerned with calculating phase diagram with THERMOCALC, the thermodynamic calculation software package for tackling mineral equilibria problems. THERMOCALC has two main components: the application itself, and the internally-consistent thermodynamic dataset it uses.

The material here relates directly to the paper providing - hopefully! - the information to allow you to reproduce the diagrams in this paper, and in the process discover how THERMOCALC works. As the material here is "frozen-in" at the time of acceptance of the paper, yet THERMOCALC and its dataset will continue to evolve, the most recent software, dataset and documentation will be available at our web sites.

The version of THERMOCALC used here is v2.6. All subsequent bug fixes and improvements will go into v2.7 et seq. The version of the thermodynamic dataset provided here is April 20, 1996. This dataset can be used, for example, for teaching purposes. However, for new research work, the most recent dataset, incorporating all the most recent calorimetric and experimental data, should be used. THERMOCALC itself is "backwards-compatible", so the newest version should normally be used regardless of which dataset is used.

The component parts of the web-based material here are available via the following links:

- [Getting started with THERMOCALC](#)
- [Running THERMOCALC](#)
- [Annotated example THERMOCALC runs](#)
- [Using Mathematica to assemble phase diagrams](#)
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THERMOCALC

Getting started

Start by downloading THERMOCALC for your computer platform (Mac or PC).

In the Mac world...

The Mac versions of THERMOCALC are in self-unstuffing archives ('thppc.sea' or 'th68k.sea') [at top level at this site]

You start by double-clicking the .sea file which then unstuffs itself. The resulting folder, on opening, should have a collection of files in it, which can be rearranged to look something like:
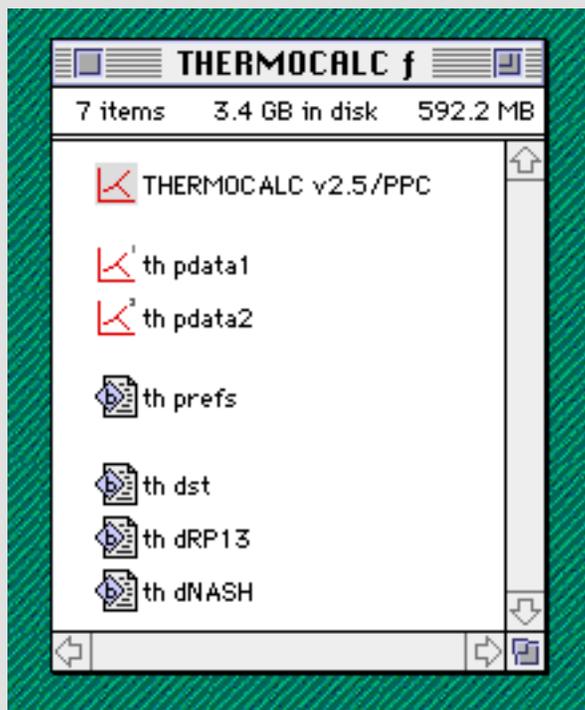
The top icon is for the application, THERMOCALC itself; the next two contain the thermodynamic dataset; the next is a preference file (that allows customisation of how THERMOCALC runs), and the last three are example datafiles (with names of the form "th dblah"). The top three icons are THERMOCALC ones; the last four are BBEdit ones - our current choice of text editor (but any text editor will do - even

the dreaded Word). (The prefs file *does* belong with the application, and not in the Preferences folder - in the System folder).

In the DOS world...

The DOS THERMOCALC is in a self-unzipping archive ('thdos.exe') [at top level at this site]

Running "thdos.exe" at a DOS prompt unzips THERMOCALC, allowing you to choose which directory the files should be placed in. In Windows95, the directory, in this case "thermo", can be arranged to look like:
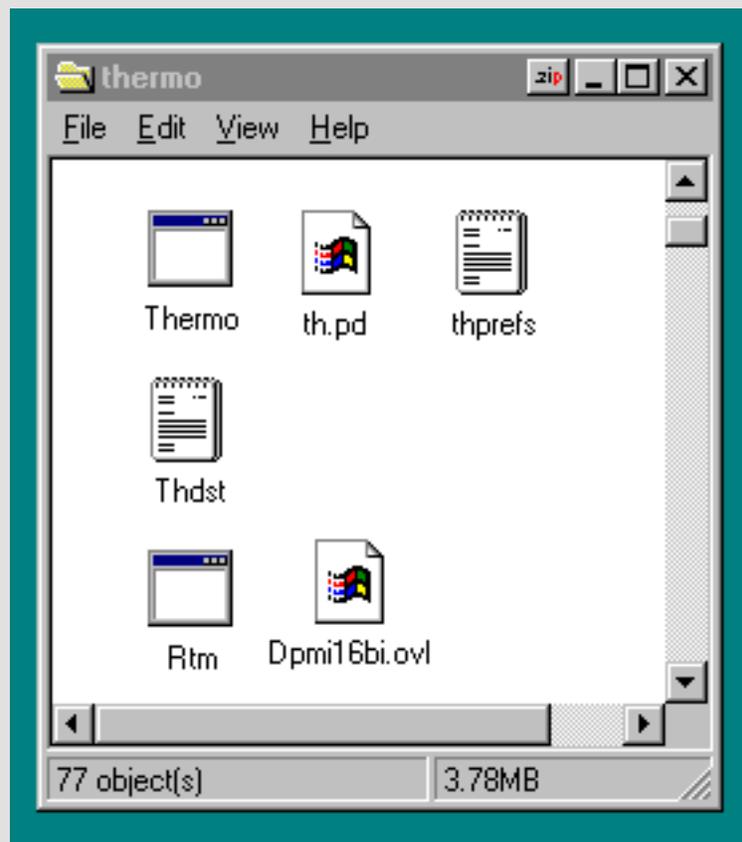
Or the directory can be handled in the normal way directly in DOS. The file namings are different from the mac version: THERMOCALC is "thermo.exe", the information in the two pdata files is in *one* file, "th.pd" (in contrast to the Mac version), and the preferences file is "thprefs.txt". Data filenames have the form "thdblah.txt", where blah is the suffix (descriptor) of your choice. The two files at

the bottom of the window are critical to the running of THERMOCALC in DOS (in DPMI: DOS Protected Mode) and must be in the same directory as "thermo.exe".

A simple THERMOCALC run

Let's do a simple run of THERMOCALC to get started. We will be running the KFMASH system because the preferences file has been configured for (a) doing phase diagram calculations (ie "calcmode 1"), and (b) these calculations are going to be done with "th dst" (DOS: "thst.dat") (ie datasuffix st). The datafile has also been configured to require little interaction from you.

- On the Mac, double-click on the THERMOCALC icon (DOS: type thermo and hit enter) to start up THERMOCALC. You will see that, even on the Mac, this a command-line type of program (no evidence of a GUI here - sorry).
- The first question you will be asked is "which phases" - hit return (DOS: enter), and this says to THERMOCALC that all phases are to be used.
- The next question you will be asked is "what variance" for the calculation. This assemblage of phases is actually invariant (defining the top of the staurolite+biotite stability field in PT - see the PT projection figure in the paper, for example), so type 0 (for variance = 0, or invariant) and hit return (DOS: enter).
- The next question you will be asked is "what PT window" for the calculation. Just hit return (DOS: enter) and the default PT window from the datafile will be used.
- Now THERMOCALC does its stuff and outputs on the screen, the PT coordinates of the invariant, as well as the compositions of all the phases in the assemblage. It also gives the calculated uncertainties on these coordinates. It also puts the info in various files, as we shall see in a moment.
- Having calculated the requested equilibrium, it then asks if you want to do any more phase diagram calculations - say no (or 0), then it asks whether you are all done - say yes or 1 or just hit return (DOS: enter). Then THERMOCALC exits (because we have "autoexit yes" in the preferences).

OK, we can now take stock. THERMOCALC has done the calculation - on screen, but what are in the output files? The file "th ost" (DOS: "thost.txt"), contains the results and sufficient of the input information for the THERMOCALC run to be understood. The logfile, "th log" (DOS: "thlog.txt"), contains much more - not only our input in response to THERMOCALC prompts, but also a human-readable representation of the phase info in the datafile. In addition "th math" (DOS: "thmath.txt") contains the PT coordinate of the invariant point in a Mathematica format.

Running THERMOCALC involves just the above sort of things:

- configuring the scripts in the preferences file,
- configuring the scripts in the datafile, and
- answering the prompts from THERMOCALC...

From here, look at

- [running THERMOCALC](#)
- [annotated THERMOCALC logfiles](#)

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THERMOCALC

The best way to find out more about running THERMOCALC is to work through the [annotated THERMOCALC logfiles](#), and actually running them yourself to make sure you can see what is going on. As it says in the [getting started](#) section, running THERMOCALC is all about

- configuring the scripts in the datafile, and
- answering the prompts from THERMOCALC

once you have the phase definitions set up in the datafile and the preferences file is configured to your liking.

For a discussion of further aspects of generating phase diagrams using THERMOCALC, look at run documentation here, in combination with the [annotated THERMOCALC logfiles](#).

Introduction

Running THERMOCALC to calculate phase diagrams involves a number of steps:

Choose a model system in which to do the calculations. A model system is just the chemical system, usually specified in terms of oxides, in which the equilibria to be calculated can be represented. This then specifies which phases, and the substitutions within them, that will be able to be considered. Obviously these phases can only involve those end-members that occur in the thermodynamic dataset (or linear combinations of those end-members). For example, the model system normally used to consider metapelites is K2O-FeO-MgO-Al2O3-SiO2-H2O (or KFMASH) (Thompson, 1957), allowing most of the critical minerals, and the FeMg(-1) and (Fe,Mg)SiAl(-1)Al(-1) (Tschermak's) substitutions in them, to be considered.

- *Generate a THERMOCALC datafile for the phases in the system.* Given that a central part of calculations on solid solutions is the calculation of the equilibrium compositions of the phases in assemblages, the datafile has to communicate to THERMOCALC the activity-composition (a-x) relationships of the phases in symbolic form, in terms of the compositional variables to be calculated.
- *Decide on which phase diagrams are to be constructed.* This decision will depend mainly on what geological problem is being addressed. Usually a key phase diagram is a P-T "projection" for the system, showing the equilibria for all bulk compositions in the model

system (possibly with a constraint on the presence of certain phases). A P-T projection for KFMASH is usually constrained by stipulating the presence of muscovite, quartz and H2O. With a P-T projection for reference, P-T "pseudosections" for example are drawn, showing just those phase relationships for particular bulk compositions in the model system. Similarly T-x and/or P-x pseudosections are drawn, showing the phase relationships for a particular bulk composition line through the model system. Some of the different phase diagram types that are possible are considered below.

- *Systematically accumulate information on stable equilibria as calculated by THERMOCALC.* This involves running all of the relevant equilibria, and then manually determining the stability relationships among them. What is involved in this should become clearer in the next section, and by following (or, better, actually running) the examples.
- Construct the phase diagram. Whereas obviously this construction can be done manually or in an appropriate graphics package, here the use of Mathematica is advocated, and a range of custom code for drawing phase diagrams is presented. THERMOCALC can write results in a Mathematica format (or, if required, in a tab-separated form).

In the following sections, there is information on calculating the main types of phase diagrams with THERMOCALC.

P-T projections

Projections are phase diagrams which show all of the invariant and univariant equilibria for all of the bulk compositions in a model system. They are the familar petrogenetic grids of the literature:
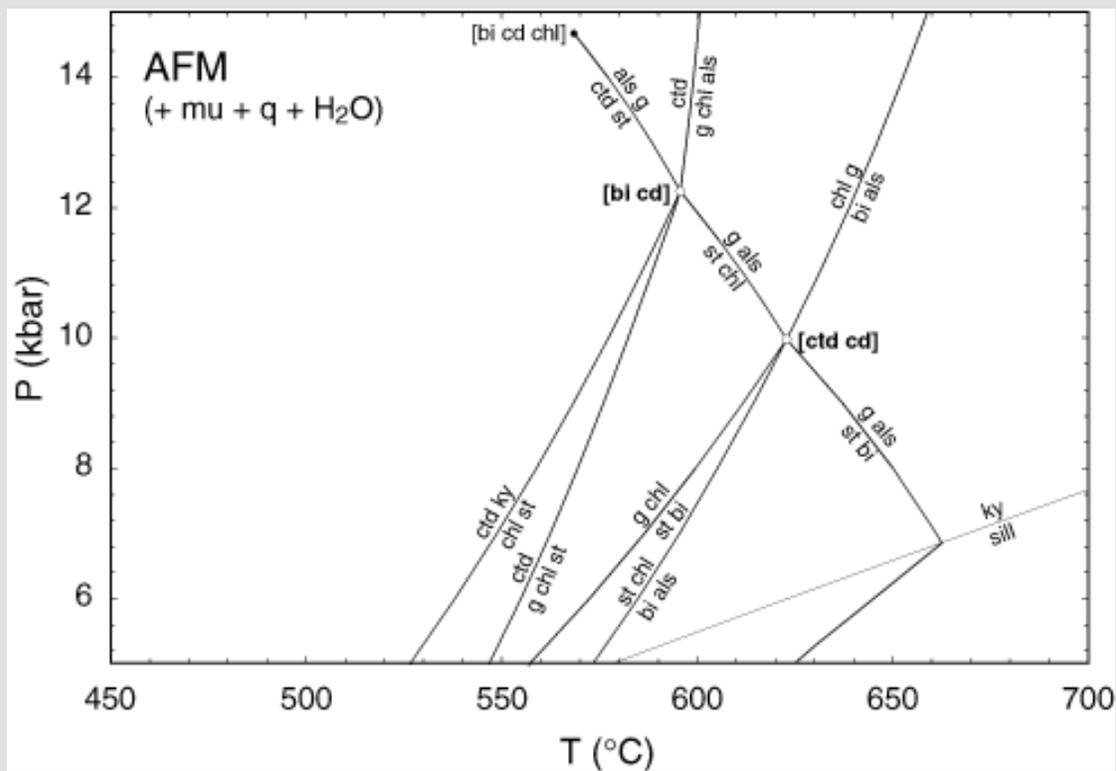
THERMOCALC output takes the form, in this case for the g+chl=st+bi univariant, the staurolite isograd reaction

```
 P(kbar)      T(°C)      x(st)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    4.0         540      0.977     0.965     0.792     0.608     0.819     0.448     0.915
0.879
        21g + 31chl + 71mu = 10st + 71bi + 117q + 104H2O
    6.0         572      0.937     0.911     0.604     0.593     0.638     0.417     0.812
0.860
        19g + 32chl + 71mu = 10st + 72bi + 115q + 112H2O
    8.0         599      0.884     0.846     0.466     0.579     0.496     0.386     0.713
0.841
        17g + 34chl + 72mu = 10st + 73bi + 114q + 118H2O
   10.0         622      0.818     0.770     0.361     0.565     0.383     0.355     0.619
0.821
        15g + 35chl + 73mu = 10st + 73bi + 113q + 123H2O
```

giving not only the PT line for the reaction, but the way the phase compositions, and the balanced chemical reaction, vary along the line.

These are the simplest diagrams to generate in that it is very easy to calculate all the invariants and univariants for a system. However, THERMOCALC does not determine the stability of equilibria. When all the univariants, for example, in a system are calculated, many or most will be metastable. The stability of the equilibria in a system can be determined by applying Schreinemakers Rule, that the metastable extension of the reaction not involving phase i (i-out or [i]) lies between i-producing reactions (eg Zen, 1966), to the univariants around each invariant,

then putting the invariants together. This process might be started in subsystems, as stable full system univariants emanate from stable subsystem invariants, eg the KFMASH univariant ctd + st = ky + g emanates from the KFASH invariant [bi,cd,chl] at high P in the above Figure. Thus, it is useful to determine the grids for KMASH and KFASH before determining the KFMASH grid.

The approach of determining the stable univariants by Schreinemaker's Rule can sometimes be short-circuited by the method illustrated in the following Table

```
no      T(°C)  inc    reaction
1        538    *     ctd + ky = st + chl
2        555    *     ctd = st + g + chl
3        557    1     ctd = st + bi + ky
4        559    1     ctd = st + g + bi
5        563    1     ctd + chl = st + bi
6        565    1     ctd = st + cd + bi
7        572    *     g + chl = st + bi
8        572    1     ctd = g + chl + ky
9        575    1     ctd = g + bi + ky
10       581    1     ctd + ky = st + cd
11       581    1     ctd + chl = bi + ky
12       583    2     g + chl = bi + ky
13       585    *     st + chl = bi + ky
14       588    1     ctd = st + cd + g
15       591    1     ctd = cd + g + ky
16       603    3     chl = st + cd + bi
17       604    1     ctd + chl = cd + g
18       604    1     ctd + bi = cd + g
19       604    1     chl = ctd + cd + bi
20       604    2     chl = cd + g + bi
21       605    1     g + chl = ctd + bi
22       619    1     st + ctd = g + ky
23       626    3     chl + ky = st + cd
24       627    2     chl + ky = cd + g
25       630    3     st + chl = cd + g
26       644    1     chl + ky = ctd + cd
27       649    2     st + chl = g + ky
28       660    5     st + cd = g + ky
29       670    *     st + bi = g + ky
30       734    4     st + bi = cd + g
```

Table 1. All the reactions at 6 kbars in KFMASH, ordered in T (except for 4 reactions that were "not in range"). The bulleted reactions are the stable ones (see text).

Here all of the univariants at a particular P are ordered in T, with each reaction written low T $\rightarrow$ high T (as given by THERMOCALC). Noting that the reaction i = j + k + l, means that i cannot be stable at higher T, so that any reaction involving i must necessarily be metastable, then reaction 2 in Table 1 excludes reactions with 1 in the "inc" column. Noting that i + j = k + l

means that i + j cannot be stable at higher T, so that any reaction involving i + j (other than with i + j alone being on the high T side of the reaction) must be metastable, then reaction 7 excludes reactions with 2 in the "inc" column, 13 excludes reactions with 3 in the "inc" column, and 29 excludes reactions with 4 in the "inc" column. The same lines of logic apply with decreasing T, so 29 also excludes reactions with 5 in the "inc" column. Thus the stable reactions in the above Table are the ones marked with a bullet (*). This method is developed here for an effective ternary system but can be generalised to apply to any size system. Note that, if certain equilibria are not found by THERMOCALC, for example for starting guess reasons, then the resulting stability relationships will be incomplete. In pathological situations (for example systems with singularities, Worley et al., 1997) disconnected i + jtrivariants may be stable, making the method difficult to apply.

Having determined the P-T projection for a system, with the establishment of the stability relationships that this entails, makes the phase diagrams of the following sections easier to calculate and draw.

Compatibility diagrams

Compatibility diagrams show the mineral assemblages, and ranges of mineral solid solutions, at a specified P-T, for all of the bulk compositions in a model system. To be useful compatibility diagrams need to involve a maximum of 3 apices (or be the equivalent orthogonal diagram), ie be an effective ternary, so that it can be represented in 2D. For this to be true usually involves a reduction in the effective size of the system by stipulating that certain phases are present in all of the equilibria being considered. The reduction of KFMASH to an effective ternary (at conditions below the upper amphibolite facies, where muscovite + quartz breaks down) is normally done by considering that muscovite, quartz and H2O are "in excess" (Thompson, 1957), and the phase relationships are projected from these phases onto Al2O3--FeO--MgO (AFM). When these projections are made, the phases must be projected from the calculated compositions of the phases involved in each equilibria (eg Thompson, 1979).
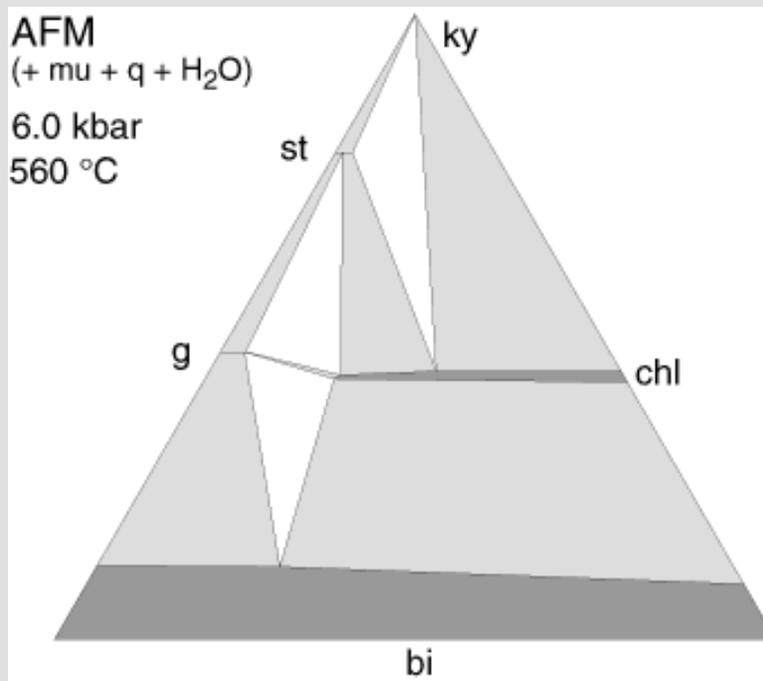
One important practical aspect of compatibility diagrams, beyond the (geological) choice of which phases to project from, is the choice of projection plane, the plane onto which the phase relationships are to be projected. It is quite reasonable for phases to plot at infinity, as does K-feldspar in AFM, but if this can be prevented it is helpful, particularly if more than one phase plots there, or if that phase is a solid solution. More seriously, the projection plane should be chosen to be between the projecting phases and the "nearest" solid solutions (Powell and Sandiford, 1987; Worley and Powell, 1997). See Worley and Powell (1997) for a discussion of this problem in relation to choosing a projection plane for NCKFMASH. In fact, the classic AFM projection for KFMASH fails at lower temperatures as a consequence of the projection plane being further away from muscovite than is biotite, for example in KAlO2--(FeO,MgO)--Al2O3. At lower temperature, on the AFM compatibility diagram, biotite in equilibrium with alkali feldspar plots at more Al-rich compositions than biotite in equilibrium with chlorite, for Fe-rich and Mg-rich compositions.

THERMOCALC is set up to calculate compatibility diagram information in a straightforward way. Having decided which phases to project from (if it is necessary), and what the compositions are of the apices of the projection plane, then the information is added to the datafile in the form of scripts. Either these scripts can be entered directly, or THERMOCALC can be run with the script "project yes" in the datafile. In this case the projection information is prompted for, and the required script information is placed in the logfile for copying into the datafile. The scripts to instruct THERMOCALC to provide AFM coordinates for the phases in each equilibrium it calculates is

```
        fluidexcess yes
        setexcess mu q
```

```
      project yes
      % [script to enter the projection plane info]
      % -------------------- Al2O3   MgO   FeO   K2O
      setproject       A          1     0     0     0
      setproject       F          0     0     1     0
      setproject yes   M          0     1     0     0
      % -------------------------------------------
```

The necessary calculations usually involve all of the divariants being calculated for the full system, giving the information for the interior of the compatibility diagram, as well as all of the divariants for the sub-systems, giving the information for the edges of the diagram. Establishing which divariants are stable can be done most easily via the relationships in the P-T projection.

THERMOCALC output takes the form, in this case for the g+chl+bi divariant

```
<====================================================>
phases : g, chl, bi, (mu, q, fluid) or [st,ky]

-------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
     6.0      560.0     0.939    0.690    0.571    0.720    0.381    0.864    0.837

proj       A        F        M       mu     phase
g       0.250    0.704    0.046            -0.250
chl     0.190    0.559    0.251            -0.167
bi     -0.228    0.871    0.356    0.500   -0.500
<====================================================>
```

with the AFM coordinates of the phases given in projection from the calculated composition of the mu.

In the AFM examples, the boundaries of the one phase fields are close to being straight lines between the apices of the tie triangles, so these boundaries are drawn as such above. In more complex systems, these boundaries can be quite curved. The easiest way to trace such trivariant-quadrivariant boundaries in compatibility diagrams is via the trivariant equilibrium and set isopleths, looking at an appropriate range of isopleths for one of the composition variables for the phase of the one phase field. For example, to trace the boundary of the chlorite one phase field on the low Al side of the above compatibility diagram, calculations on the trivariant, chl-bi(-mu-q-H2O), with x(chl) set to say 0 through to 0.75 at 0.05 intervals, will give the coordinates of the ends of the tie lines between biotite and chlorite. As well as defining the low Al side of the chlorite one phase field, this will give the high Al side of the biotite one phase field.

In complex systems, for example the NCKFMASH system considered by Worley et al. (1997), the reduction of the system so that it is effective ternary requires considering five phases to be in excess (eg plagioclase, biotite, muscovite, quartz and H2O). There comes a point when such

reductions cannot be done in a useful way. Further, such reductions may conceal more than they reveal if projected bulk compositions migrate too much with changing conditions. This can happen if most of the mode of the bulk composition is being projected from, particularly if projection from several solid solutions is involved. In this case, it is likely that an x-x pseudosection, showing the phase relationships for a bulk composition plane through the system, would be more useful. Such diagrams can be calculated with THERMOCALC, but not in a straightforward way.

P-T pseudosections

A P-T pseudosection is a P-T diagram on which just the phase relationships that apply to (or are "seen" by) a specified bulk composition are shown. In the same way that a compatibility diagram can have one phase (quadrivariant), two phase (trivariant), and three phase (divariant) fields, so can P-T pseudosections. In addition, P-T pseudosections can involve those parts of a P-T projection which are seen by the bulk composition: univariant lines and invariant points.
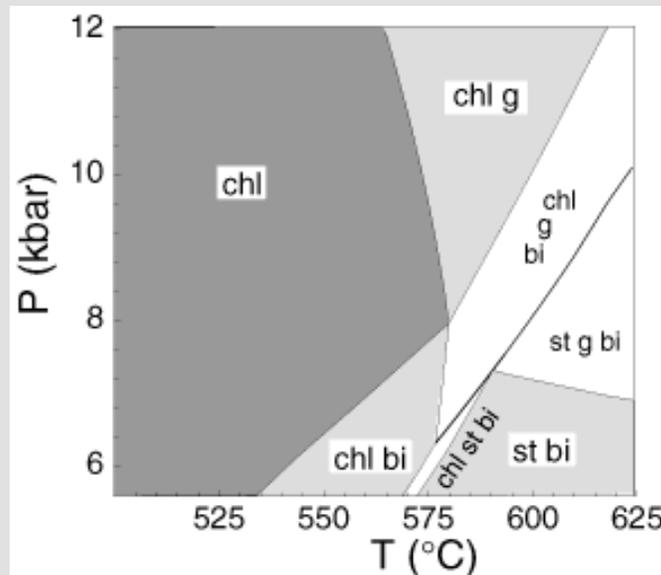
To access pseudosection facilities in THERMOCALC, the "pseudosection" script in the datafile must be set. Then, running THERMOCALC, the user is prompted for the bulk composition that is to be used. A bulk composition could, for example, be derived from a whole rock analysis, or be an estimated equilibration volume composition constructed from the analysed compositions of phases in an assemblage. This bulk composition appears in the logfile in an appropriate form, and can be copied across to the datafile. The script to instruct THERMOCALC to provide pseudosection information with the bulk composition used in the examples is

```
pseudosection yes
% [script to enter the bulk composition info]
```

```
       % ----------- Al2O3    MgO    FeO    K2O ---------
       setbulk yes   41.89  18.19  27.29  12.63
       % -------------------------------------------------
       setmodeiso yes
       zeromodeiso yes
```

The latter two scripts access a facility that is central to calculating pseudosections. Various points and lines on pseudosections can be understood in terms of particular modes going to zero (so "zeromodeiso"). For example, in the above Figure, the lower P extent of the univariant is where the modes of g and st go to zero. The notation used for a such a point is chl bi (st g), indicating that the equilibrium involves all four phases, but with the modes of the phases in brackets set to zero. It can be calculated, using the above script, by specifying the univariant equilibrium and specifying that the modes of g and st are set to zero at the appropriate prompt in THERMOCALC. All the points and lines in the above Figure are calculated in this way (apart from the univariant lines and invariant points). Note that on such pseudosections, variance changes by 2 between the highest and lowest variance fields at points.

THERMOCALC output takes the form, in this case for the bi chl (st g) point that terminates the seen part of the g+chl=st+bi univariant as it goes into the bi+chl trivariant

```
Al2O3    MgO    FeO    K2O
 41.89  18.19  27.29  12.63
<====================================================>
phases : st, g, chl, bi, (mu, q, fluid)

 P(kbar)      T(°C)     x(st)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    6.31      576.8    0.9292    0.9014    0.5797    0.5906    0.6134    0.4120    0.7962
0.8573

   mode        st        g       chl        bi        mu
              0         0    0.4439    0.1019    0.4543
<====================================================>
```

with the PT coordinate of the point given, as well as the modes of the phases that apply at the point.

The usual procedure followed when constructing a P-T pseudosection is to start by plotting the chosen bulk composition on compatibility diagrams for a series of P-T conditions corresponding to those of the pseudosection. This indicates which mineral assemblages, ie which fields, should be expected. Then the stable univariants are examined; where a univariant is seen, the modes of the divariants either side of the reaction are given. Along the reaction, changes in the divariant seen indicate the crossing of a trivariant termination on the univariant. Such terminations can then be calculated directly. Then the resulting divariant-trivariant boundariescan be followed by calculating the divariant with the mode of the appropriate phase set to zero. Looking at chl bi (g),

the mode of bi progressively decreases up P, eventually going to zero: this is chl (g bi), the corner where the chl quadrivariant terminates against the divariant. The corner is calculated by specifying the divariant and setting the modes of g and bi to zero. So P-T pseudosections are built up, each point and line at a time, once the parts of the stable univariants that are seen have been determined.

Note that divariants, in particular, can be very narrow. As a consequence care is needed, meaning that a very fine P or T step may be needed in looking at univariants, to ensure that narrow divariants are not missed. Once identified, the width of a divariant does not affect the calculation of its boundaries, as they are specified separately in terms of the modes that go to zero there, in going into the adjacent trivariants.

Although the stability relationships can usually be established directly from those in the PT projection---specifically in providing a starting point from which a pseudosection can grow---sometimes, particularly if no part of a stable univariant is seen by the bulk composition, an alternative is needed. This is provided by a Gibbs energy minimisation facility in which all the possible assemblages seen by the bulk composition are calculated. The stable one is the one of lowest Gibbs energy. Such output is:

P(kbar)	T(°C)	st	g	chl	bi	mu	ky	q	H2O	var
9.0	565	–	–	*	–	*	–	*	*	4
9.0	570	–	–	*	–	*	–	*	*	4
9.0	575	–	–	*	–	*	–	*	*	4
9.0	580	–	*	*	–	*	–	*	*	3
9.0	585	–	*	*	–	*	–	*	*	3
9.0	590	–	*	*	–	*	–	*	*	3
9.0	595	–	*	*	*	*	–	*	*	2
9.0	600	–	*	*	*	*	–	*	*	2
9.0	605	–	*	*	*	*	–	*	*	2
9.0	610	–	*	*	*	*	–	*	*	2
9.0	615	*	*	–	*	*	–	*	*	2
9.0	620	*	*	–	*	*	–	*	*	2

Table 2. Gibbs energy minimisation by looking at the Gibbs energies of all divariant, trivariant and quadrivariant equilibria at 9 kbar and 565 through to 620^\circC for the bulk composition: mol% Al2O3 = 41.89, mol% MgO =18.19, mol% FeO = 27.29, and mol% K2O = 12.63 calculated by THERMOCALC.

T-x and P-x pseudosections

A f(P,T)-x pseudosection is a diagram on which the phase relationships that apply to (or are "seen" by) a specified bulk composition line along a P-T line (ie f(P,T)) through the model system are shown. Normally such a pseudosection is drawn at constant P, making it a T-x pseudosection, or at constant T, making it a P-x pseudosection. In the following, for simplicity,

they will be described in terms of a T-x pseudosection as the logic and approach are equivalent for both. For example:
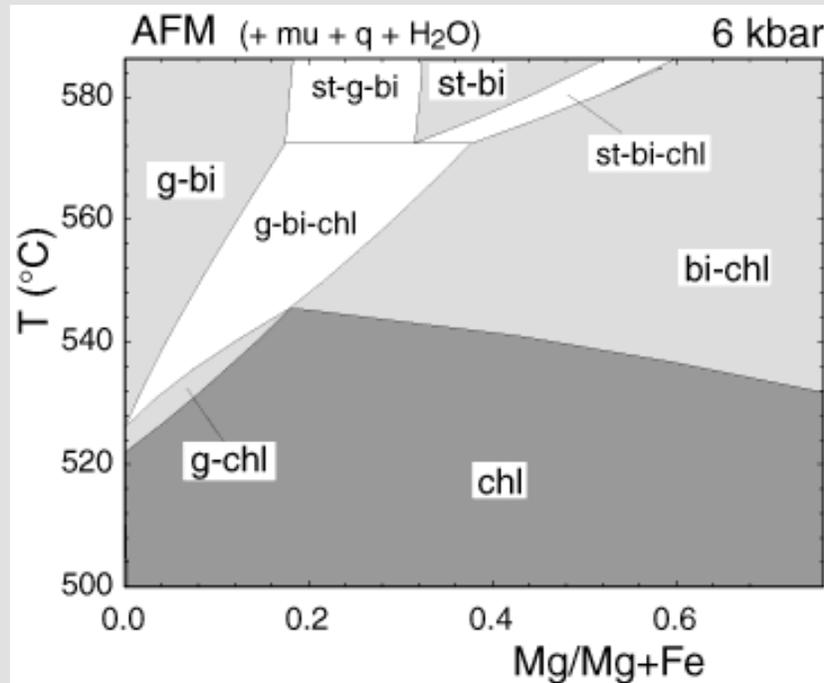
In the same way that a P-T pseudosection can have one phase (quadrivariant), two phase (trivariant), and three phase (divariant) fields, so can T-x pseudosections. On T-x pseudosections univariant (and invariant) equilibria occur as horizontal lines whose length is controlled by the range of bulk compositions along the composition line that "see" the equilibria.

To access these pseudosection facilities in THERMOCALC, the "pseudosection" script in the datafile must be set. Then, running THERMOCALC, the user is prompted for the ends of a bulk composition line that is to be used. Alternatively, a composition line can be generated from a single bulk composition used, for example, in a P-T pseudosection, by for example varying Fe--Mg through that composition. For example, using the bulk composition from the previous section as a basis for exploration of Fe-Mg variation, the scripts to instruct THERMOCALC to provide pseudosection information are

```
pseudosection yes
% [script to enter the bulk composition info]
% ----------- Al2O3   MgO     FeO    K2O ----------
setbulk yes   41.89  45.48      0  12.63
setbulk yes   41.89      0  45.48  12.63
% ---------------------------------------------------
setmodeiso yes
zeromodeiso yes
```

In the previous bulk composition, $MgO = 18.19$ and $FeO = 27.29$; adding these gives 45.48, so the bulk composition line extends from $MgO = 45.48$ and $FeO = 0$, to $MgO = 0$ and $FeO = 45.48$.

The same approach is followed in constructing a T-x pseudosection as in constructing a P-T pseudosection, with the main difference being that any calculation is repeated for each bulk composition. As before, the stable univariants are examined first, looking to see the composition range, if any, over which a univariant is seen. As in the P-T case, the modes of the divariants either side of the reaction are given for each bulk composition seen. The T-x pseudosection is built up in the same way as for the P-T pseudosection by following divariant-trivariant lines, recognising the existing of qudrivariant fields, following the trivariant-quadrivariant boundaries, and so on. One difference arises in the calculation of points in that THERMOCALC calculates the trace of such a point with varying P, and the user must interpolate to get the T and x values for the fixed P of the pseudosection.

Again, note that fields can be very narrow. As a consequence, small sections of the bulk composition line may need to be examined in looking at univariants, to ensure that narrow divariants are not missed.

From here, look at

- [annotated THERMOCALC logfiles](#)

or go back to

- [getting started](#)

[[back to beginning](#)]

Annotated THERMOCALC logfiles

AFM examples

In looking at the logfiles accessed from this page, there are certain conventions that are followed. Commentary is in green; annotation is in blue; what is produced by THERMOCALC is in black (and datafile material); and user input is in red. (Somtimes, when it looks as though a THERMOCALC prompt has been answered by the user, and so should be in red, it is in black because the question has been answered via a script). Look at

- [PT projection calculations](#)
- [Projection calculations](#)
- [Isopleth calculations](#)
- [Generating bulk compositions.](#)
- [PT pseudosection calculations](#)
- [Tx pseudosection calculations](#)
- [Gibbs energy minimisation](#)
- [Uncertainty calculations](#)

as well as

- [AFM datafile and scripts](#)
- [Abbreviations and formulae](#)
- [Reaction coefficients](#)
- [Singularities](#)

[[back to the start](#)]

Annotated THERMOCALC logfiles

PT projection calculations

In this example we will calculate some of the features of a PT projection, showing the positions of invariant points and univariant lines.

These calculations are for KFMASH with muscovite, quartz and H2O taken to be in excess (ie AFM), so in the discussion in the following assemblages will only be given in terms of the AFM phases, with the additional presence of mu, q and H2O always being understood. These excess phases are clearly present in the THERMOCALC output.
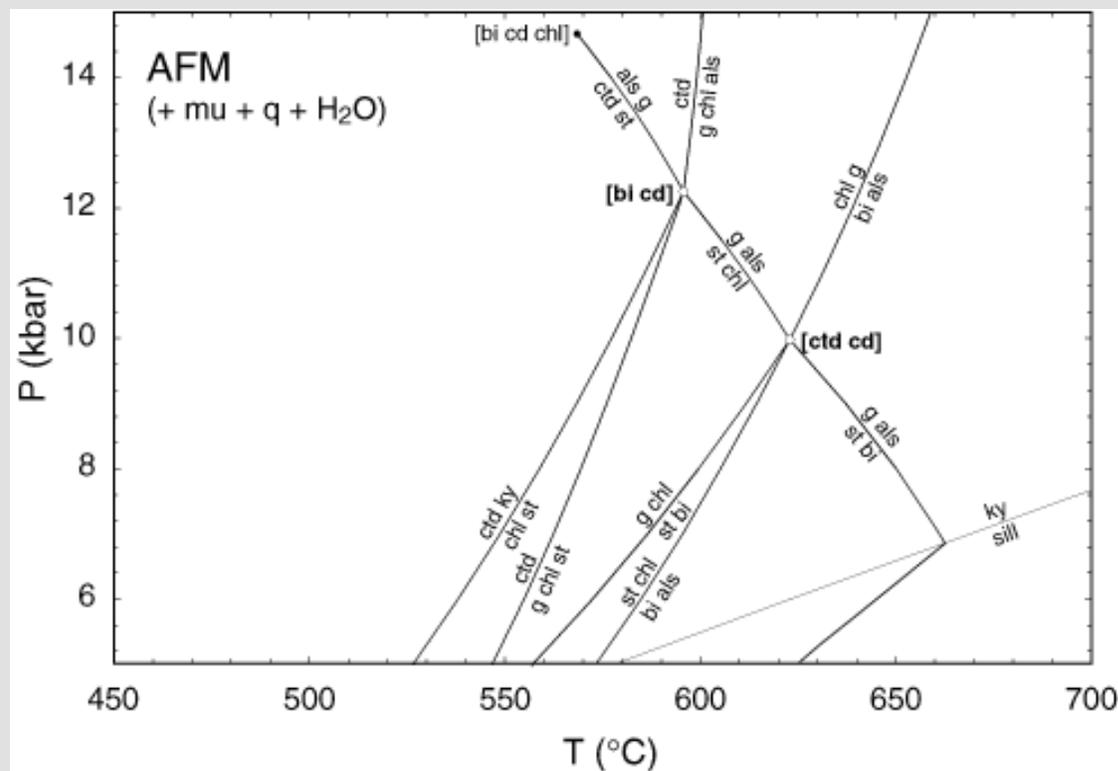
This figure is the finished PT projection, for reference, calculated with THERMOCALC.

Invariant point

We wish to calculate the P and T of the invariant AFM assemblage g+chl+st+ky+bi and the compositions of the minerals in the assemblage.

```
THERMOCALC v2.5, © Roger Powell and Tim Holland running at 18.35 on Thu 5 Dec,1996
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
```

```
calculation type :
      0 = table of thermodynamic data of end-members
      1 = phase diagram calculations
      2 = average pressure-temperature calculations
      3 = calculations on all reactions between end-members
      4 = list end-member names and compositions
control code  : 1
```

means do mode 1 phase diagram calculations

```
data filename : suffix to "th d" : st
```

filename to use is "th dst"

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O

log output will be found in "th log" (from prefs)
output will be found in the file, "th ost" (from prefs)
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
output will be found in the file, "th math" (from prefs)

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases : (nothing input)
```

expecting a list of phases to use; hitting return (without entering anything) means use all of the phases.
(Entering "all" means the saem, as obviously does typing in the whole list).

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 0
```

means we want to calculate an invariant point (invariant = 0)

```
specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high :  300 1000 5 15
```

set the PT window within which the invariant point is expected to occur. (We could have just hit return here,
and the default PT window in the datafile would have been used).

```
<=================================================>
phases : st, g, chl, bi, ky, (mu, q, fluid)
reactions : |XXX|XX|XXX|XX
 P(kbar)     T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
    10.0       622     0.819    0.771    0.362    0.565    0.385    0.356    0.620
0.822
```

In the output above, the first line is a list of the phases involved in the equilibrium, with excess phases in parentheses. The second line is a record of the calculation of an independent set of reactions (The x's represent the 10 independent reactions needed to determine the 10 unknowns - P, T and the 8 compositional variables whose values are listed).

```
more phase diagram calculations ? yes
```

so continue

Emanating from an invariant point like the one we have just calculated will be a set of univariant reactions, one for each phase involved in the invariant point. We would normally not draw the reactions not involving mu, q or H2O (ie [mu], [q] or [H2O]), because these phases are taken to be in excess (ie always present) in AFM calculations. We will look at the staurolite isograd reaction (g+chl+mu = st+bi+q+H2O) at pressures between 3 and 6 kbar, ie at [ky].

Univariant reaction

We calculate the temperature of the univariant staurolite isograd reaction (g+chl+mu = st+bi+q+H2O) at pressures between 3 and 6 kbar, as well as determine the compositions of all phases along the reaction boundary

continuing from above

```
data filename : suffix to "th d" : st
```

filename to use is "th dst"

```
reading phase info from this file ...
st ctd cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O
=================================================

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky
```

this time we want to calculate the ky-absent reaction

```
fluid is in excess (from script)

use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance : 1
```

means calculate a univariant equilibrium

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :  3 10
```

calculate temperatures for pressures between 3 and 10 kbar

```
T window within which reactions expected to lie
T window: T low,high :  300 1000
```

the T window in which calculated T's are expected to lie. (Just hitting return here would mean that the default T window set in the datafile would be used)

```
P window :3 <-> 10 kbar :P interval : 1
```

calculate temperatures at 1 kbar intervals

```
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions : |XX|X|X|XXX|XX
```

P(kbar)	T(°C)	x(st)	x(g)	x(chl)	y(chl)	x(bi)	y(bi)	x(mu)	y(mu)
3.0	522	0.992	0.988	0.916	0.616	0.929	0.463	0.968	0.888

```
        23g + 29chl + 70mu = 10st + 71bi + 118q + 99H2O
```

P(kbar)	T(°C)	x(st)	x(g)	x(chl)	y(chl)	x(bi)	y(bi)	x(mu)	y(mu)
4.0	540	0.977	0.965	0.792	0.608	0.819	0.448	0.915	0.879

```
        21g + 31chl + 71mu = 10st + 71bi + 117q + 104H2O
```

P(kbar)	T(°C)	x(st)	x(g)	x(chl)	y(chl)	x(bi)	y(bi)	x(mu)	y(mu)
5.0	557	0.958	0.940	0.690	0.600	0.723	0.433	0.863	0.870

```
        20g + 32chl + 71mu = 10st + 72bi + 116q + 108H2O
```

P(kbar)	T(°C)	x(st)	x(g)	x(chl)	y(chl)	x(bi)	y(bi)	x(mu)	y(mu)
6.0	572	0.937	0.911	0.604	0.593	0.638	0.417	0.812	0.860

```
        19g + 32chl + 71mu = 10st + 72bi + 115q + 112H2O
```

```
   7.0        586     0.912     0.880     0.530     0.586     0.563     0.401     0.762
0.851
       17g + 33chl + 72mu = 10st + 72bi + 114q + 115H2O
   8.0        599     0.884     0.846     0.466     0.579     0.496     0.386     0.713
0.841
       17g + 34chl + 72mu = 10st + 73bi + 114q + 118H2O
   9.0        611     0.852     0.809     0.411     0.572     0.436     0.370     0.666
0.831
       16g + 35chl + 72mu = 10st + 73bi + 113q + 120H2O
  10.0        622     0.818     0.770     0.361     0.565     0.383     0.355     0.619
0.821
       15g + 35chl + 73mu = 10st + 73bi + 113q + 123H2O
```

In the output above, THERMOCALC has calculated the 8 x's and y's plus T, at the fixed P of each calculation. It did this by solving the equilibrium relationships for the 9 independent reactions that can be written between the end-members of these phases: 15 end-members minus 6 components (KFMASH) gives 9 independent reactions.

Note that the compositions of all the phases in the reaction assemblage are becoming more magnesian to higher P, but with the same order of Fe:Mg, as reflected in the x value = Fe/(Fe+Mg).

At each pressure the reaction is written in balanced form, using the actual calculated compositions of the phases, so the reaction coefficients vary along the reaction line.

more phase diagram calculations ? yes

To determine the stability of the univariants such as this one around the invariant point we calculated, we use Schreinemakers analysis: that the metastable extension of [i] lies between i-producing reactions. Having calculated all the univariants around the invariant, we see that the reaction we have just calculated [ky] is stable to lower P, where we have calculated it.

To calculate all the reactions around this invariant, at the question "which phases", we just hit return, and THERMOCALC then loops through all the possible univariants that can be written between the phases.

Although not strictly relevant to a calculation of a PT projection, we now calculate one of the divariants adjacent to the staurolite isograd reaction.

Divariant field

In this example we wish to calculate the compositions of garnet, biotite and staurolite in the divariant AFM assemblage g+st+bi just above the staurolite isograd at some fixed PT point, e.g. 6 kbar, 580°C.

continuing from above

```
data filename : suffix to "th d" : st
```

filename to use is "th dst" (or "thst.dat" in DOS)

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O
=======================================================

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky chl
```

this time we want to omit the phases ky and chl.

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance : 2
```

the equilibrium we want is divariant

```
specification of PT window:
P range over which equilibria to be calculated
P window: P low,high : 6
```

Only one pressure in (kbar) entered. For a range in P, two pressures would need to be entered here, and you would then be prompted for the P interval to be used

```
T range over which equilibria to be calculated
T window: T low,high : 580
```

Again, only one temperature in °C. We are only interested in 6kbar, 580°C. For a range in T, two temperatures would need to be entered here, and you would then be prompted for the interval

```
<=====================================================>
phases : st, g, bi, (mu, q, fluid)
reactions : |X|XXX|XX
 P(kbar)      T(°C)     x(st)     x(g)     x(bi)     y(bi)     x(mu)     y(mu)
     6.0      580.0     0.934     0.907     0.632     0.423     0.807     0.862
```

In the output above, there are 6 x's representing the 6 independent reactions needed to determine the 6 unknowns at fixed P and T (the 6 compositional variables whose values are listed).

more phase diagram calculations ? no

no, no more mode 1 calculations

all done ? yes

yes, finished with using THERMOCALC

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THERMOCALC with Mathematica

Generating phase diagrams

THERMOCALC does not produce graphics itself. The main reason for this is that generalising the work of turning THERMOCALC output into graphics is not currently feasible. On the other hand, it is relatively straightforward to do this with an external graphics engine - we use Mathematica for this purpose - and a minimum amount of human intervention assembling the THERMOCALC output.

There are currently two levels for doing this

- lower level functions, requiring more human intervention, but suitable for the rapid generation of single diagrams. In this case, the cleaning up and labelling of a diagram would be done in, say, Adobe Illustrator. (Mathematica can 'export' graphics in Adobe Illustrator format). Look at

  drawline functions
  drawing a PT projection
  drawing a compatibility diagram
  drawing a PT pseudosection
  drawing a Tx pseudosection
- higher level functions, requiring less human intervention, suitable for generating diagrams over a range of conditions, for example in producing all the frames of an animation (phase diagram ``movies''). Look at the Mathematica files (in pdf)

  AFM compatibility diagrams at 3 kbar
  AFM compatibility diagrams at 6 kbar

  And look at the Mathematica files (in pdf)

[AFM T-x pseudosection at a range of pressures](#)
[AFM P-x pseudosection at 600°C](#)
[AFM T-y pseudosection at 6 kbars](#)

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THERMOCALC with Mathematica

lower level functions: drawline etc

drawline is a Mathematica function to draw a line on a diagram. The function is passed: a matrix of information, info, of which the ycol column is to be plotted against the xcol column, from start to *end*. If xinfo is True, start and end refer to the part of the line to be drawn in terms of the horizontal (x) axis; otherwise they refer to the y axis. start and/or end may be specified in terms of the x and y coordinate of the point, if, for example, it is an invariant point. See below for examples of its use. The point of the drawline function is that it interpolates the input data, and also incorporates the end-points in the interpolation, if they are provided as {x,y} points.

```
drawline[info_, xcol_,ycol_, xinfo_, start_,end_] :=

   Module[{os,oe,ii,x,y,if,r1,r2,o1,o2,inca,n,inc,osub,vsub},
      os = If[Length[start]==0,start,start[[If[xinfo,1,2]]]];
      oe = If[Length[end]==0,end,end[[If[xinfo,1,2]]]];

      ii = Map[#[[{xcol,ycol}]]&,info];
      If[Length[start] == 2, AppendTo[ii,start]];
      If[Length[end] == 2, AppendTo[ii,end]];
      {x,y} = Transpose[Sort[ii]];

      If[xinfo, {o,v} = {x,y}; {olow,ohigh} = {xlow,xhigh},
               {v,o} = {x,y}; {olow,ohigh} = {ylow,yhigh}];

      if = Interpolation[Transpose[{o,v}]];
      {r1,r2} = Apply[List,if][[1]];

      {oo1,oo2} = If[oe > os,{If[os > r1, os, r1],If[oe < r2, oe, r2]},
                            {If[oe > r1, oe, r1],If[os < r2, os, r2]}];
      {o1,o2} = {If[oo1 > olow,  oo1, olow], If[oo2 < ohigh, oo2, ohigh]};

      If[o2 < o1,  Line[{}],
         inca = (ohigh - olow)/nop;
         n = Round[(o2 - o1)/inca]; If[n < 4, n = 4];
         inc = (o2 - o1)/n;

         osub = Range[o1,o2,inc]; vsub = Map[if[#]&,osub];
```

```
        Line[Transpose[If[xinfo, {osub,vsub}, {vsub,osub}]]] ]  /;

     Length[Dimensions[info]]==2 && Dimensions[info][[2]]>1;

drawline[___] := (Print["wrong shape, or data defines a point"];{});
```

outline function

The function, outline, just draws the box into which drawline draws lines.

```
outline := {AbsoluteThickness [0.3], GrayLevel[0],
         Line[{{xlow, ylow},{xlow, yhigh},
              {xhigh, yhigh},{xhigh, ylow},{xlow, ylow}}]};
```

compatibility diagram functions

Simple functions for plotting compatibility diagrams; in particular, tri plots a tie triangle, and one plots a one-phase field. conv and close are utilities used by tri and one.

```
rsqrt3 = 1/Sqrt[3];  ll = 1.36;   lla = ll rsqrt3;

conv[s_] := N[{rsqrt3(s[[4]] - s[[3]]), -(s[[4]] + s[[3]])}];
close[p_] := Line[Join[p,{p[[1]]}]];
tri[t_] := close[Map[conv, t[[2]]]];
one[w_] := close[Map[(conv[#[[1,2,#[[2]]]]])&, w]];
```

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THERMOCALC with Mathematica

PT projection using drawline function

THERMOCALC is run in the normal way, as in the log runs, with the "makeo yes" (and "ofilename th math") in the preferences file, and the "smath yes" script in the datafile. Then coordinate information is put into "th math" as well as onto screen and into the other files by THERMOCALC. This coordinate information is in Mathematica form (in curly brackets), with annotation also in Mathematica form - as (* ... *). In the following table, the data has been assembled, and more particularly 'named', so that it can be used in the drawline code. The naming can be in any user-defined way - here an 'out'-way has been used (so bioutpt can be read as "[bi] point", and so on).

The invariant info is given in x (horizontal), y (vertical) axis order

```
(*  Invariants *)

bioutpt =    {595.6, 12.25};                    (* [bi]  *)
ctdoutpt =   {622.9, 9.98};                     (* [ctd] *)
```

The univariant info is given in the order that it is presented in "th math", and drawline orders it for drawing (via the "..., 2, 1, ..." coding in the drawline calls)

```
(*  Univariants *)

bigout =                                  (*  [bi,g]  *)
    {{6.00, 537.9},{8.00, 558.8},{10.00, 577.3},
     {12.00, 593.7},{14.00, 608.4}};

bikyout =                                 (*  [bi,ky]  *)
    {{6.00, 554.9},{8.00, 569.4},{10.00, 582.3},
     {12.00, 594.2},{14.00, 605.6}};

bichlout =                                (*  [bi,chl]  *)
    {{6.00, 618.9},{8.00, 618.5},{10.00, 611.4},
```

```
             {12.00, 597.8},{14.00, 577.2}};

bistout =                              (*  [bi,st]  *)
     {{6.00, 571.9},{8.00, 582.0},{10.00, 589.5},
      {12.00, 595.1},{14.00, 599.1}};

bictdout =                             (*  [bi,ctd]  *)
     {{6.00, 649.0},{8.00, 639.5},{10.00, 622.7},
      {12.00, 599.0},{14.00, 568.7}};

ctdstout =                             (*  [ctd,st]  *)
     {{6.00, 582.5},{8.00, 604.5},{9.00, 614.2},
      {11.00, 631.3},{12.00, 638.9},{14.00, 652.7}};

ctdchlout =                            (*  [ctd,chl] *)
     {{6.00, 670.0},{8.00, 650.1},{10.00, 622.6},
      {12.00, 588.7},{14.00, 549.0}};

ctdgout =                              (*  [ctd,g]  *)
     {{6.00, 584.8},{8.00, 605.2},{9.00, 614.4},
      {11.00, 631.3},{12.00, 639.2},{14.00, 654.1}};

ctdkyout =                             (*  [ctd,ky]  *)
     {{6.00, 572.4},{8.00, 599.6},{10.00, 623.1},
      {12.00, 643.8},{14.00, 662.3}};
```

These variables just define an outer PT window within which the drawing window is located.

```
tlow = 0; thigh = 1000; plow = 0; phigh = 50;
```

These variables define the drawing window. Once the following graphics calls are sorted out, drawing in a new window is as simple as putting different numbers in here.

```
xlow = 520; xhigh = 670; ylow = 6; yhigh = 14;
```

This call of Show[...] assembles the graph. The outline call returns the drawing box to Graphics, then there is a drawline call - which returns to Graphics the line to be drawn - for each of the named equilibria above. Each drawline call involves: the name of the line; the x,y axis positions in the info - "..., 2, 1, ..." (ie x is the

2nd position; y is the 1st position); "...,True, ..." that y is interpolated in x (normal, unless the line has a minimum or a maximum in it); and the last two are the plotting range of the line (either in terms of the outer window, or in terms of an {x,y} point)

```
Show[Graphics[{outline,
            drawline[bigout,    2,1, True,  tlow, bioutpt],
            drawline[bikyout,   2,1, True,  tlow, bioutpt],
            drawline[bichlout,  2,1, True,  tlow, bioutpt],
            drawline[bistout,   2,1, True,  bioutpt, thigh],
            drawline[bictdout,  2,1, True,  bioutpt, ctdoutpt],
            drawline[ctdstout,  2,1, True,  ctdoutpt, thigh],
            drawline[ctdchlout, 2,1, True,  ctdoutpt, thigh],
            drawline[ctdgout,   2,1, True,  tlow, ctdoutpt],
            drawline[ctdkyout,  2,1, True,  tlow, ctdoutpt]}],
    AspectRatio -> 1, Frame -> True,
    PlotRange -> {{xlow, xhigh}, {ylow, yhigh}} ];
```
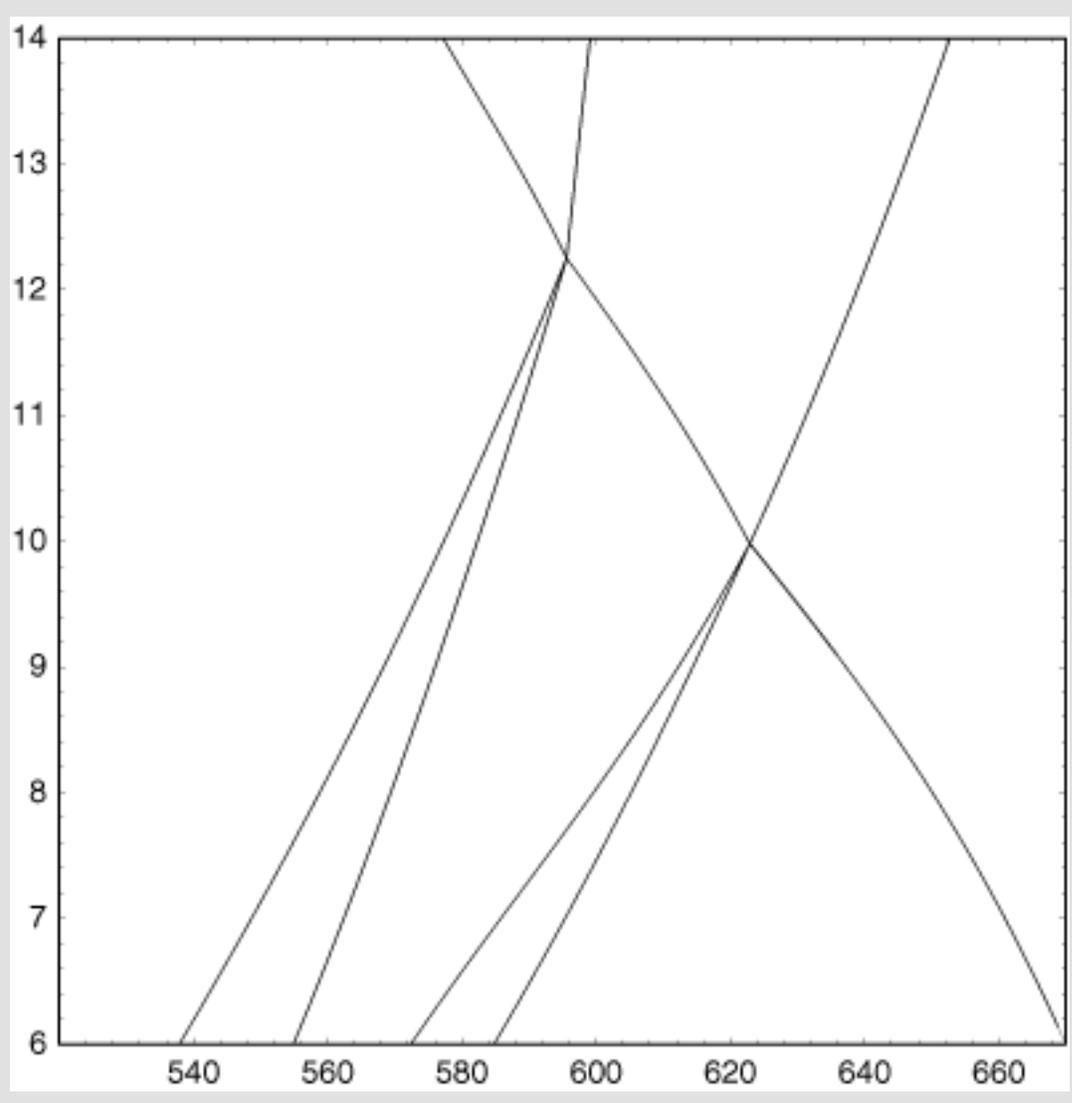
and for reference
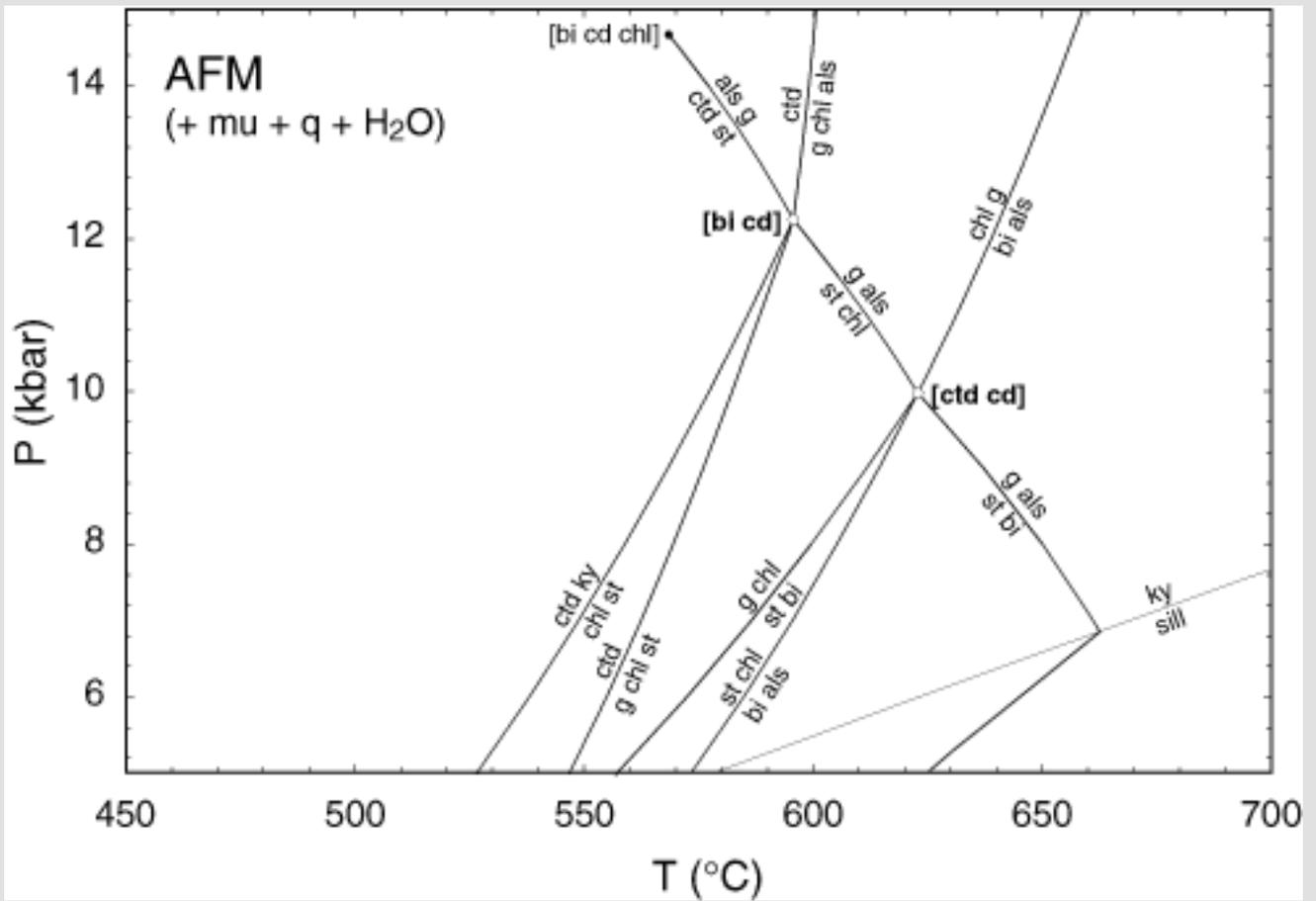
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THERMOCALC with Mathematica

compatibility diagram using one, tri...

THERMOCALC is run in the normal way, as in the log runs, with the "makeo yes" (and "ofilename th math") in the preferences file, and the "cmath yes" script in the datafile. Then coordinate information is put into "th math" as well as onto screen and into the other files. This coordinate information is in Mathematica form (in curly brackets), with annotation also in Mathematica form - as (* ... *). In the following table, the data has been assembled, and more particularly 'named', so that it can be used in the simple code following. The naming can be in any user-defined way.

Coordinate information produced by THERMOCALC, named in terms of the phases involved

```
(*  AFM coordinates  *)

stgchl = {{6.000, 560.00},
         {{"st", 0.6923, 0.2938, 0.0139},
          {"g", 0.2500, 0.7016, 0.0484},
          {"chl", 0.1985, 0.5428, 0.2587}} };

stchlky = {{6.000, 560.00},
         {{"st", 0.6923, 0.2742, 0.0335},
          {"chl", 0.2071, 0.3557, 0.4373},
          {"ky", 1.0000, 0, 0}} };

gchlbi = {{6.000, 560.00},
         {{"g", 0.2500, 0.7042, 0.0458},
          {"chl", 0.1904, 0.5586, 0.2510},
          {"bi", -0.2275, 0.8714, 0.3561}} };

(*  AF coordinates (zero column added)  *)

gstFe = {{6.000, 560.00},
         {{"g", 0.2500, 0.7500, 0},
          {"st", 0.6923, 0.3077, 0}} };

stkyFe = {{6.000, 560.00},
         {{"st", 0.6923, 0.3077, 0},
          {"ky", 1.0000, 0, 0}} };

bigFe = {{6.000, 560.00},
         {{"bi", -0.3003, 1.3003, 0},
```

```
                  {"g", 0.2500, 0.7500, 0}} };

(*   AM coordinates (zero column added)   *)

bichlMg = {{6.000, 560.00},
          {{"bi", -0.3578, 0, 1.3578},
           {"chl", 0.1830, 0, 0.8170}} };

chlkyMg = {{6.000, 560.00},
          {{"chl", 0.2071, 0, 0.7929},
           {"ky", 1.0000, 0, 0}} };

(*  biotite bottom edge *)

bilimFe = {{}, {{"bi",-0.4, 1.4,    0}}};
bilimMg = {{}, {{"bi",-0.4,   0, 1.4}}};
```

Call of Show[...] assembles the compatibility diagram. The tri (tie triangle) calls just take the tie triangle coordiante info. The one calls take the defining tie triangles, with an index for the position in the tie triangle info that is to be used.

```
Show[Graphics[{Line[{{-lla,-ll}, {0,0}, {lla,-ll}}],
               tri[stgchl], tri[stchlky], tri[gchlbi],
               one[{{bichlMg,2},{gchlbi,2},{stgchl,3},{stchlky,2},{chlkyMg,1}}],
               one[{{stkyFe,1},{stchlky,1}}],
               one[{{bigFe,2},{stgchl,2}}],
               one[{{bilimFe,1},{bigFe,1},{gchlbi,3},{bichlMg,1},{bilimMg,1}}] }],
      AspectRatio->Automatic];
```

and for reference

AFM
(+ mu + q + H_2O)
6.0 kbar
560 °C

ky

st

g

chl

bi
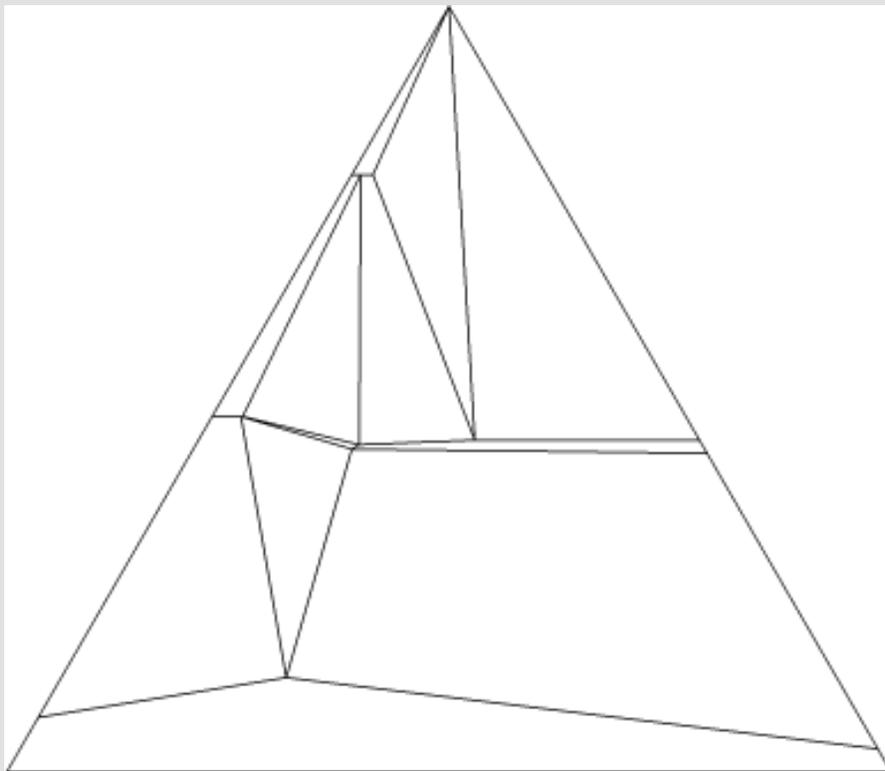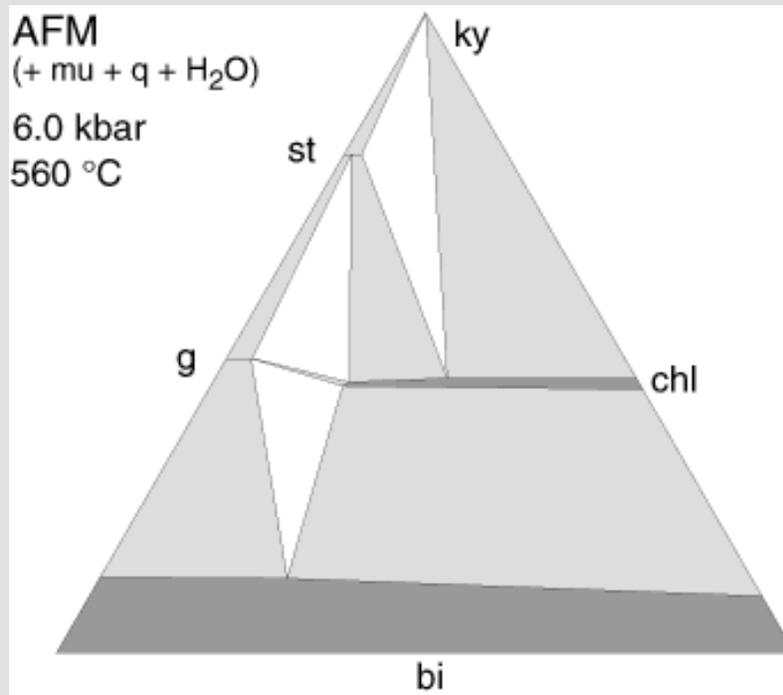
[back one | back to beginning]

THERMOCALC with Mathematica

PT pseudosection using drawline function

The use of drawline in this example is much like that in the PT projection example above. The equilibria have been named in terms of the phases involved - see the Mathematica annotation in each case.

```
inpt1 = Reverse[{9.97, 622.1}];                    (*  st g chl bi ky  invariant *)

kyout =                                            (*  g chl = st bi  univariant *)
   {{5.00, 557.1},{6.00, 572.3},{7.00, 586.3},{8.00, 599.3},
    {9.00, 611.3}, {10.00, 622.5},{11.00, 633.0}};

kyoutchlbi = Reverse[{6.31, 576.8}];               (*  chl bi (st g) di corner on
univariant *)
kyoutstbi = Reverse[{7.30, 590.3}];                (*  st bi (g chl) di corner on
univariant *)

chlbi =                                            (*  chl (bi)  quadrivariant edge *)
   {{3.00, 479.5},{4.00, 500.7},{5.00, 521.3},
    {6.00, 541.4},{7.00, 561.3}, {8.00, 580.9}};

chlg =                                             (*  chl (g)  quadrivariant edge *)
   {{7.00, 581.6},{8.00, 579.8},{9.00, 577.1},{10.00, 573.6},
    {11.00, 569.4},{12.00, 564.6},{13.00, 559.3},{14.00, 553.5}};

qpt = Reverse[{7.95, 579.9}];                      (*  chl (g bi)  corner of
quadrivariant *)

chlbig =                                           (*  chl bi (g)  divariant edge *)
   {{3.00, 563.4},{4.00, 569.2},{5.00, 573.2},
    {6.00, 576.1},{7.00, 578.2}};

gchlbi =                                           (*  g chl (bi)  divariant edge *)
   {{9.00, 590.0},{10.00, 599.5},{11.00, 608.6},
    {12.00, 617.3},{13.00, 625.4}, {14.00, 633.0}};

chlbist =                                          (*  chl bi (st)  divariant edge *)
   {{3.00, 536.9},{4.00, 550.5},{5.00, 562.6},
    {6.00, 573.6},{7.00, 583.7},{8.00, 593.3}};

stbichl =                                          (*  st bi (chl)  divariant edge  *)
   {{3.00, 541.0},{4.00, 554.6},{5.00, 566.6},
    {6.00, 577.4},{7.00, 587.4},{8.00, 596.8}};

stbig =                                            (*  st bi (g)  divariant edge  *)
   {{5.00, 813.2},{6.00, 703.1},{7.00, 614.5},
```

```
    {8.00, 536.6},{9.00, 465.0},{10.00, 395.2}};
```

Drawing window

```
xlow = 550; xhigh = 620; ylow = 5; yhigh = 11;
```

The call of Show[...] assembles the diagram.

```
Show[Graphics[{outline,
             drawline[chlbi,       2,1, True,  tlow, qpt],
             drawline[chlg,        2,1, False, qpt, phigh],
             drawline[kyout,       2,1, True,  kyoutchlbi,inpt1],
             drawline[chlbist,     2,1, True,  tlow, kyoutchlbi],
             drawline[chlbig,      2,1, True,  kyoutchlbi, qpt],
             drawline[gchlbi,      2,1, True,  qpt, thigh],
             drawline[stbichl,     2,1, True,  tlow, kyoutstbi],
             drawline[stbig,       2,1, True,  kyoutstbi, thigh]}],
     AspectRatio -> 1, Frame -> True,
     PlotRange -> {{xlow, xhigh}, {ylow, yhigh}} ];
```
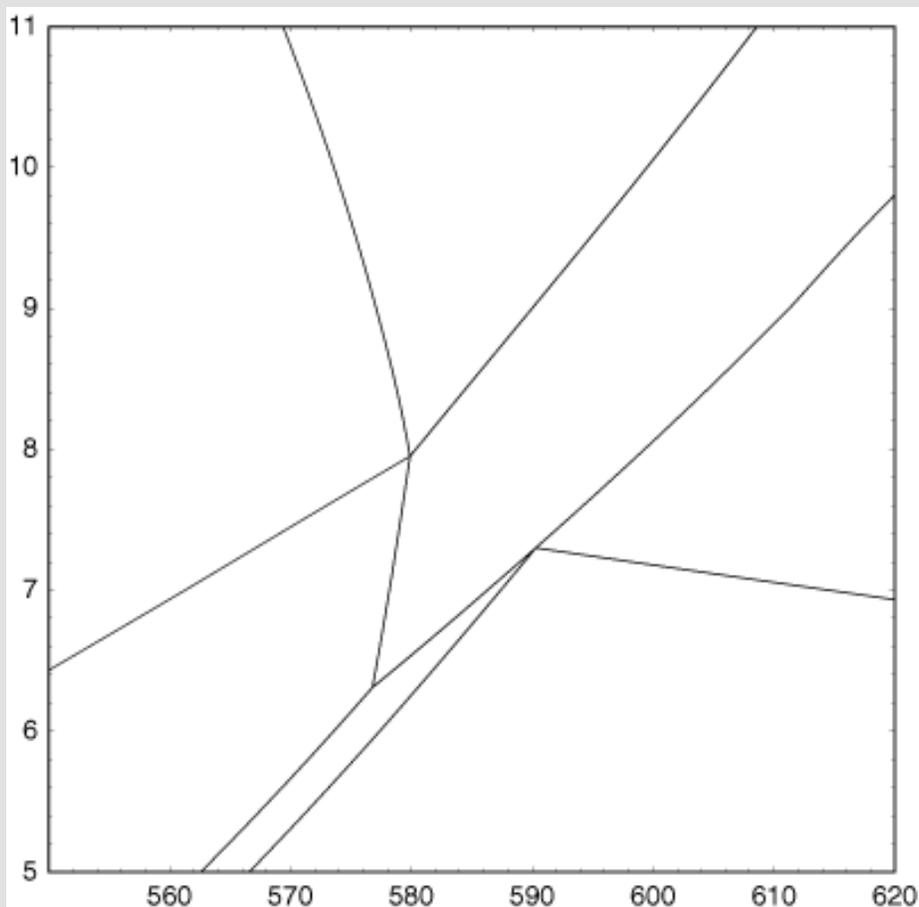
and for reference
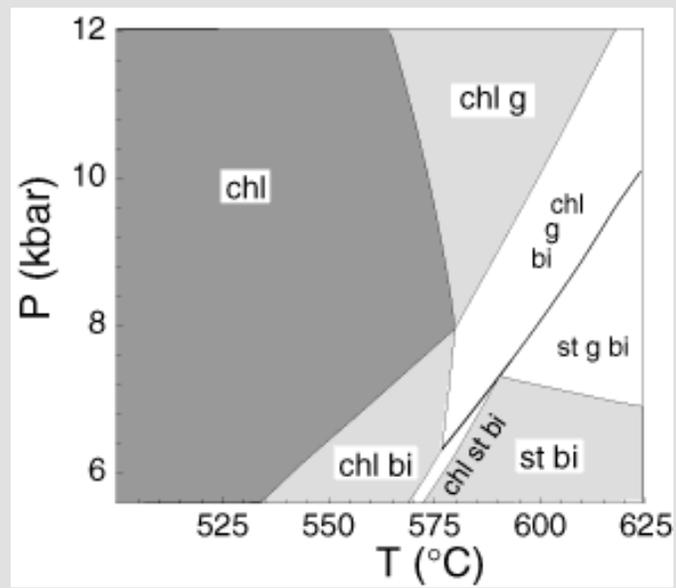
[back one | back to beginning]

THERMOCALC with Mathematica

T-x pseudosection using drawline function

The use of drawline in this example is much like that in the PT projection and PT pseudosection examples above. The equilibria have been named in terms of the phases involved - see the Mathematica annotation in each case. The form of the THERMOCALC output produced is a little different in this case because the bulk composition information is also needed.

```
gbichl = {{ 0.0000, 6.00, 526.0, {"g", "bi"},"chl"},
           { 0.0400, 6.00, 538.6, {"g", "bi"},"chl"},
           { 0.0800, 6.00, 549.3, {"g", "bi"},"chl"},
           { 0.1200, 6.00, 559.3, {"g", "bi"},"chl"},
           { 0.1600, 6.00, 568.9, {"g", "bi"},"chl"}};

gchlbi = {{      0, 6.00, 526.0, {"g", "chl"},"bi"},
           { 0.0400, 6.00, 531.6, {"g", "chl"},"bi"},
           { 0.0800, 6.00, 536.1, {"g", "chl"},"bi"},
           { 0.1200, 6.00, 540.1, {"g", "chl"},"bi"},
           { 0.1600, 6.00, 543.7, {"g", "chl"},"bi"}};

chlbig = {{ 0.1800, 6.00, 545.4, {"chl", "bi"},"g"},
           { 0.2200, 6.00, 550.4, {"chl", "bi"},"g"},
           { 0.2600, 6.00, 555.6, {"chl", "bi"},"g"},
           { 0.3000, 6.00, 561.0, {"chl", "bi"},"g"},
           { 0.3400, 6.00, 566.8, {"chl", "bi"},"g"}};

chlbist ={{ 0.3500, 6.00, 571.1, {"chl", "bi"},"st"},
           { 0.4000, 6.00, 573.6, {"chl", "bi"},"st"},
           { 0.4500, 6.00, 576.4, {"chl", "bi"},"st"},
           { 0.5000, 6.00, 579.3, {"chl", "bi"},"st"},
           { 0.5500, 6.00, 582.5, {"chl", "bi"},"st"},
           { 0.6000, 6.00, 585.8, {"chl", "bi"},"st"}};

stbichl ={{ 0.3000, 6.00, 571.5, {"st", "bi"},"chl"},
           { 0.3500, 6.00, 574.5, {"st", "bi"},"chl"},
           { 0.4000, 6.00, 577.5, {"st", "bi"},"chl"},
```

```
          {  0.4500,  6.00,  580.8,  {"st",  "bi"},"chl"},
          {  0.5000,  6.00,  584.2,  {"st",  "bi"},"chl"},
          {  0.5500,  6.00,  587.8,  {"st",  "bi"},"chl"}};

gbist =  {{  0.1800,  6.00,  580.3,  {"g",  "bi"},"st"},
          {  0.2000,  6.00,  610.9,  {"g",  "bi"},"st"},
          {  0.2200,  6.00,  641.2,  {"g",  "bi"},"st"}};

stbig =  {{  0.3200,  6.00,  578.6,  {"st",  "bi"},"g"},
          {  0.3400,  6.00,  607.5,  {"st",  "bi"},"g"},
          {  0.3600,  6.00,  637.8,  {"st",  "bi"},"g"}};

chlg =   {{       0,  6.00,  521.8,  {"chl"},"g"},
          {  0.0400,  6.00,  526.7,  {"chl"},"g"},
          {  0.0800,  6.00,  531.7,  {"chl"},"g"},
          {  0.1200,  6.00,  537.1,  {"chl"},"g"}};

chlbi =  {{  0.3200,  6.00,  543.0,  {"chl"},"bi"},
          {  0.4900,  6.00,  539.4,  {"chl"},"bi"},
          {  0.6600,  6.00,  534.5,  {"chl"},"bi"},
          {  0.8300,  6.00,  528.0,  {"chl"},"bi"},
          {  1.0000,  6.00,  519.2,  {"chl"},"bi"}};

qpt = {0.1780, 545.2};

unigbi = {0.173, 572.4};
unistbi = {0.315, 572.4};
unichlbi = {0.375, 572.4};
```

The outer window (for T) and the drawing window

```
tlow = 0; thigh = 1000;
xlow = 0; xhigh = 0.6; ylow = 520; yhigh = 585;
```

The call of Show[...] assembles the diagram.

```
Show[Graphics[{outline,
             drawline[chlg,    1,3, True, 0, qpt],
             drawline[chlbi,   1,3, True, qpt, 1],
             drawline[gbichl,  1,3, True, 0, unigbi],
             drawline[gchlbi,  1,3, True, 0, qpt],
             drawline[chlbig,  1,3, True, qpt, unichlbi],
             drawline[gbist,   1,3, True, unigbi, 1],
```

```
            drawline[stbig,    1,3, True, unistbi, 1],
            drawline[stbichl, 1,3, True, unistbi, 1],
            drawline[chlbist, 1,3, True, unichlbi,1],
            Line[{unigbi,unichlbi}]}],
    AspectRatio -> 1, Frame -> True,
    PlotRange -> {{xlow, xhigh}, {ylow, yhigh}} ];
```
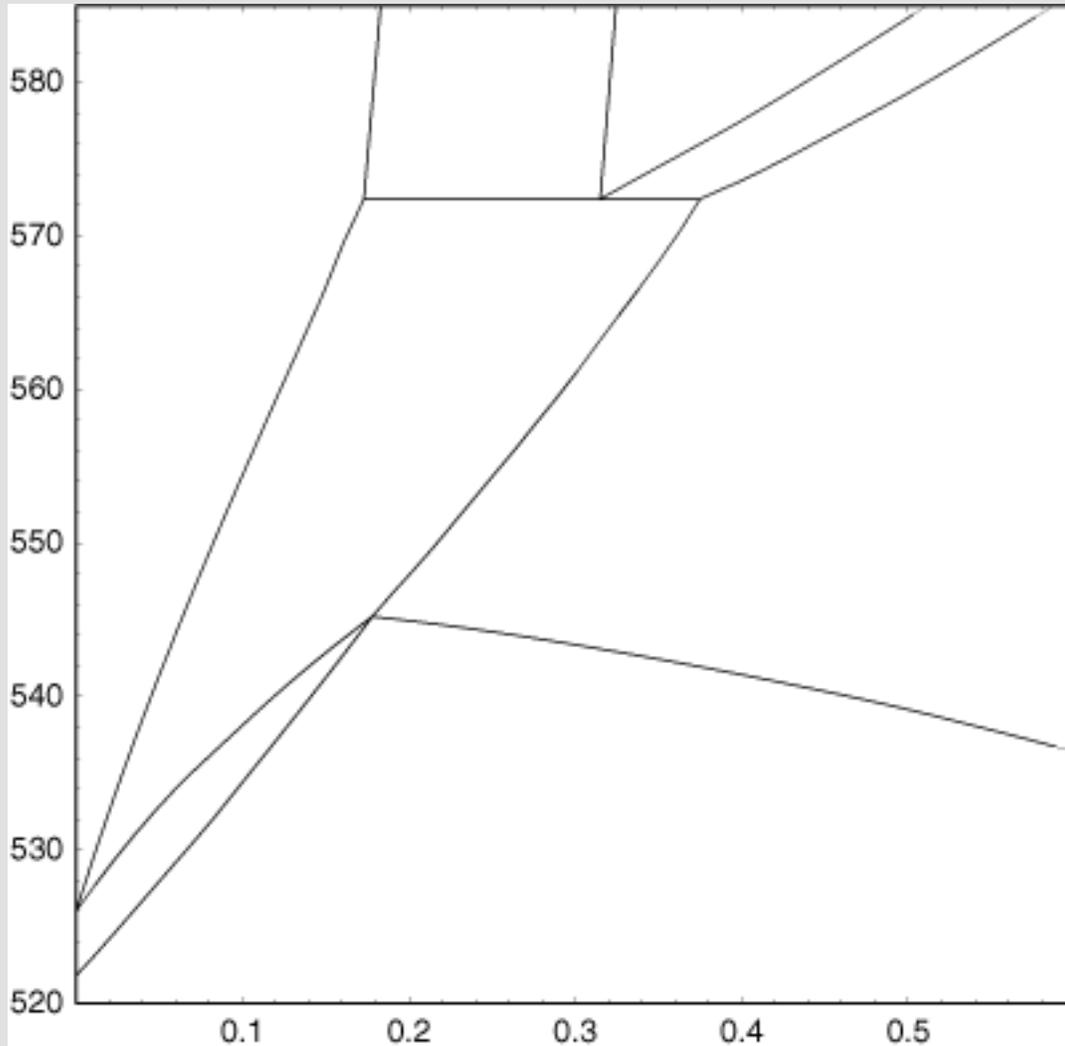
and for reference
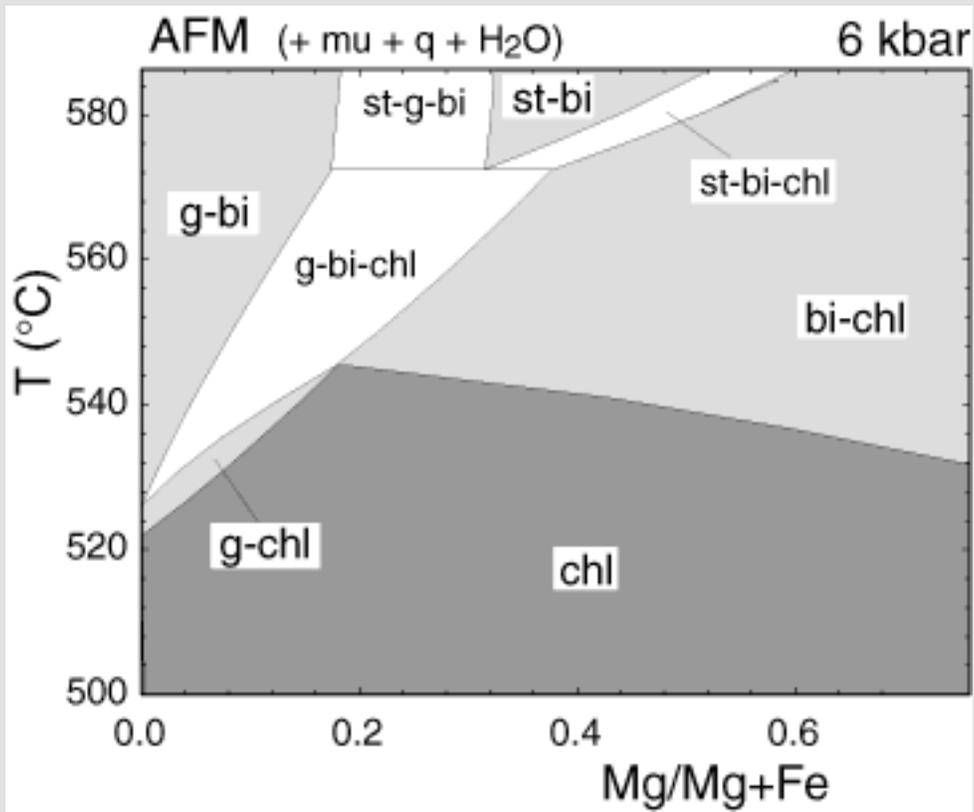
[back one | back to beginning]

■ AFM compatibility diagrams at 3 kbar

■ AFM system-specific functions

applies function f to AFM coordinates as provided by THERMOCALC,
after converting them into graphical coordinates

```
Clear[conv];
conv[f_,t_]:=(p = Map[(Mg = #[[4]]; Fe = #[[3]];
                      N[ {(Mg - Fe)/Sqrt[3], -(Mg + Fe)} ] )&, t];
              f[Join[p,{p[[1]]}]]);

conv[t_]:= (Mg = t[[4]]; Fe = t[[3]]; N[ {(Mg - Fe)/Sqrt[3], -(Mg + Fe)} ]);
```

---

default font sizes

```
fontsize1 = 12; fontsize = 16;

varyTatP = True;
```

---

creates AFM triangle (triangle not joined up, so no bottom line on triangle)

```
third = 1/3;        sqrtthird = 1/Sqrt[3];      twothird = 2/3;

ll = 1.36; lla = ll sqrtthird;
cll = 1 - ll; clla = 1 - cll;
dd = 0.03;

{xky,yky} = {0,0}; xbot = lla + dd sqrtthird; ybot = -ll - dd;

shape = N[{{-xbot,ybot}, {0,0}, {xbot,ybot}}]

{{-0.802517, -1.39}, {0, 0}, {0.802517, -1.39}}
```

---

plot range info

```
xband = 0.191; yband = 0.05;     (* for AspectRatio -> Automatic *)

xlow0 = -xbot - xband; xhigh0 = xbot + xband;
ylow0 = ybot - yband; yhigh0 = yband;

plotrange = {{xlow0,xhigh0},{ylow0,yhigh0}};
plotrangef = plotrange;
```

---

default slider coordinates

```
y = -1.6; dy = 0.02; dy1 = 0.05;
x1 = -0.8; x2 = 0.8;
yplus = 0.032; yminus = -0.075;
```

---

vscale

```
xsc = -0.77; ysc = -0.32; pl = 1;

plotvscale[v_] := Text[FontForm[N[Round[10^pl v]/10^pl],
                                {"Helvetica",fontsize}], {xsc,ysc},{-1,0}]
```

---

draws labels

```
Clear[labelling];
labelling[p_] :=
    ({Text[FontForm[p,{"Helvetica",fontsize}], {-0.7,-0.21}],
     Text[FontForm["AFM",{"Times-Bold",18}], {-0.7,-0.1}],
     Text[FontForm["als",{"Helvetica",fontsize}], {0.1,-0.05}],
     Text[FontForm["st",{"Helvetica",fontsize}], {-0.27,-0.3}],
     Text[FontForm["ctd",{"Helvetica",fontsize}], {-0.38,-0.5}],
     Text[FontForm["g",{"Helvetica",fontsize}], {-0.52,-0.75}],
     Text[FontForm["chl",{"Helvetica",fontsize}], {0.54,-0.80}],
     Text[FontForm["bi",{"Helvetica",fontsize}], {0,-1.33}]});
```

---

assembly of data

```
Clear[assemble];
assemble[tk_] :=
    (infok = interpolatedi[phase, info, tk];
     infosubfk = Map[Map[Insert[#, 0,-1]&, #]&,
                     interpolatedi[phasesubf, infosubf, tk]];
     infosubmk = Map[Map[Insert[#, 0, 3]&, #]&,
                     interpolatedi[phasesubm, infosubm, tk]];
     allinfo = Join[infok,infosubfk,infosubmk]);
```

■ **coordinates**

☐ **divariants**

KFM coordinates

```
phase = {"chl","bi","g","st","ctd","and"};

equivalence = {};

info = {
{{3.000,  480.00},
        {{"ctd", 0.5000, 0.3956, 0.1044},
         {"chl", 0.2251, 0.4173, 0.3576},
         {"and", 1.0000, 0, 0}} },

{{3.000,  491.81},
        {{"ctd", 0.5000, 0.4084, 0.0916},
         {"chl", 0.2216, 0.4542, 0.3241},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3077, 0.0000},
         {"ctd", 0.5000, 0.5000, 0.0000},
         {"and", 1.0000, 0, 0}} },

{{3.000,  510.52},
        {{"st", 0.6923, 0.2955, 0.0122},
         {"chl", 0.2163, 0.5169, 0.2669},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2955, 0.0122},
         {"ctd", 0.5000, 0.4283, 0.0717},
         {"and", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.4283, 0.0717},
         {"chl", 0.2163, 0.5169, 0.2669},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2955, 0.0122},
         {"ctd", 0.5000, 0.4283, 0.0717},
         {"chl", 0.2163, 0.5169, 0.2669}} },

{{3.000,  511.26},
        {{"st", 0.6923, 0.2954, 0.0123},
         {"chl", 0.2161, 0.5160, 0.2679},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2959, 0.0118},
         {"ctd", 0.5000, 0.4305, 0.0695},
         {"chl", 0.2158, 0.5240, 0.2603}},

        {{"ctd", 0.5000, 0.5000, 0.0000},
         {"chl", 0.1988, 0.8012, 0.0002},
         {"bi", -0.2206, 1.2206, 0.0000}} },
```

{{3.000, 516.45},
        {{"st", 0.6923, 0.2947, 0.0130},
         {"chl", 0.2146, 0.5105, 0.2749},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2987, 0.0090},
         {"ctd", 0.5000, 0.4459, 0.0541},
         {"chl", 0.2121, 0.5750, 0.2129}},

        {{"ctd", 0.5000, 0.4888, 0.0112},
         {"chl", 0.2017, 0.7462, 0.0521},
         {"bi", -0.2174, 1.1487, 0.0687}},

        {{"ctd", 0.5000, 0.5000, 0.0000},
         {"g", 0.2500, 0.7500, 0.0000},
         {"bi", -0.2171, 1.2171, 0.0000}} },

{{3.000, 523.98},
        {{"st", 0.6923, 0.2937, 0.0140},
         {"chl", 0.2126, 0.5024, 0.2850},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3022, 0.0054},
         {"ctd", 0.5000, 0.4668, 0.0332},
         {"chl", 0.2069, 0.6531, 0.1400}},

        {{"st", 0.6923, 0.3077, 0.0000},
         {"ctd", 0.5000, 0.5000, 0.0000},
         {"g", 0.2500, 0.7500, 0.0000}},

        {{"ctd", 0.5000, 0.4876, 0.0124},
         {"g", 0.2500, 0.7426, 0.0074},
         {"bi", -0.2123, 1.1379, 0.0744}},

        {{"ctd", 0.5000, 0.4716, 0.0284},
         {"chl", 0.2058, 0.6722, 0.1220},
         {"bi", -0.2124, 1.0498, 0.1626}} },

```
{{3.000, 524.91},
        {{"st", 0.6923, 0.3027, 0.0050},
         {"chl", 0.2063, 0.6631, 0.1306},
         {"bi", -0.2117, 1.0373, 0.1744}},

        {{"st", 0.6923, 0.3027, 0.0050},
         {"ctd", 0.5000, 0.4693, 0.0307},
         {"bi", -0.2117, 1.0373, 0.1744}},

        {{"ctd", 0.5000, 0.4693, 0.0307},
         {"chl", 0.2063, 0.6631, 0.1306},
         {"bi", -0.2117, 1.0373, 0.1744}},

        {{"st", 0.6923, 0.3027, 0.0050},
         {"ctd", 0.5000, 0.4693, 0.0307},
         {"chl", 0.2063, 0.6631, 0.1306}},

        {{"st", 0.6923, 0.2936, 0.0141},
         {"chl", 0.2123, 0.5015, 0.2862},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3066, 0.0011},
         {"ctd", 0.5000, 0.4930, 0.0070},
         {"g", 0.2500, 0.7458, 0.0042}},

        {{"ctd", 0.5000, 0.4861, 0.0139},
         {"g", 0.2500, 0.7416, 0.0084},
         {"bi", -0.2117, 1.1285, 0.0832}} },

{{3.000, 526.12},
        {{"st", 0.6923, 0.3051, 0.0026},
         {"g", 0.2500, 0.7404, 0.0096},
         {"bi", -0.2109, 1.1164, 0.0944}},

        {{"st", 0.6923, 0.3051, 0.0026},
         {"ctd", 0.5000, 0.4840, 0.0160},
         {"bi", -0.2109, 1.1164, 0.0944}},

        {{"ctd", 0.5000, 0.4840, 0.0160},
         {"g", 0.2500, 0.7404, 0.0096},
         {"bi", -0.2109, 1.1164, 0.0944}},

        {{"st", 0.6923, 0.3051, 0.0026},
         {"ctd", 0.5000, 0.4840, 0.0160},
         {"g", 0.2500, 0.7404, 0.0096}},

        {{"st", 0.6923, 0.2934, 0.0143},
         {"chl", 0.2120, 0.5002, 0.2878},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3016, 0.0061},
         {"chl", 0.2067, 0.6400, 0.1532},
         {"bi", -0.2114, 1.0059, 0.2055}} },
```

```
{{3.000, 526.96},
        {{"st", 0.6923, 0.3051, 0.0026},
         {"g", 0.2500, 0.7402, 0.0098},
         {"bi", -0.2106, 1.1150, 0.0956}},

        {{"st", 0.6923, 0.3008, 0.0069},
         {"chl", 0.2070, 0.6242, 0.1688},
         {"bi", -0.2112, 0.9840, 0.2272}},

        {{"st", 0.6923, 0.2933, 0.0144},
         {"chl", 0.2117, 0.4994, 0.2889},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.0000, 0.5000},
         {"chl", 0.2118, 0.0000, 0.7882},
         {"and", 1.0000, 0, 0}} },

{{3.000, 534.75},
        {{"st", 0.6923, 0.2922, 0.0155},
         {"bi", -0.2086, 0.7966, 0.4120},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2922, 0.0155},
         {"chl", 0.2096, 0.4916, 0.2988},
         {"and", 1.0000, 0, 0}},

        {{"chl", 0.2096, 0.4916, 0.2988},
         {"bi", -0.2086, 0.7966, 0.4120},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2922, 0.0155},
         {"chl", 0.2096, 0.4916, 0.2988},
         {"bi", -0.2086, 0.7966, 0.4120}},

        {{"st", 0.6923, 0.3047, 0.0030},
         {"g", 0.2500, 0.7388, 0.0112},
         {"bi", -0.2078, 1.1019, 0.1060}},

        {{"cd", 0.5000, 0.1394, 0.3606},
         {"chl", 0.2097, 0.2618, 0.5285},
         {"and", 1.0000, 0, 0}} },
```

```
{{3.000, 537.75},
        {{"cd", 0.5000, 0.1969, 0.3031},
         {"bi", -0.2119, 0.5992, 0.6127},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.1969, 0.3031},
         {"chl", 0.2088, 0.3596, 0.4316},
         {"and", 1.0000, 0, 0}},

        {{"chl", 0.2088, 0.3596, 0.4316},
         {"bi", -0.2119, 0.5992, 0.6127},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.1969, 0.3031},
         {"chl", 0.2088, 0.3596, 0.4316},
         {"bi", -0.2119, 0.5992, 0.6127}},

        {{"st", 0.6923, 0.3045, 0.0032},
         {"g", 0.2500, 0.7382, 0.0118},
         {"bi", -0.2068, 1.0967, 0.1101}},

        {{"st", 0.6923, 0.2931, 0.0146},
         {"bi", -0.2075, 0.8150, 0.3925},
         {"and", 1.0000, 0, 0}} },

{{3.000, 538.50},
        {{"st", 0.6923, 0.3045, 0.0032},
         {"g", 0.2500, 0.7380, 0.0120},
         {"bi", -0.2065, 1.0953, 0.1112}},

        {{"st", 0.6923, 0.2933, 0.0144},
         {"bi", -0.2072, 0.8195, 0.3877},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.1973, 0.3027},
         {"bi", -0.2117, 0.6003, 0.6113},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.0000, 0.5000},
         {"chl", 0.2018, 0.0000, 0.7988},
         {"bi", -0.2311, 0.0000, 1.3525}} },

{{3.000, 572.28},
        {{"st", 0.6923, 0.3026, 0.0051},
         {"bi", -0.1950, 1.0426, 0.1525},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3026, 0.0051},
         {"g", 0.2500, 0.7313, 0.0187},
         {"and", 1.0000, 0, 0}},

        {{"g", 0.2500, 0.7313, 0.0187},
         {"bi", -0.1950, 1.0426, 0.1525},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3026, 0.0051},
         {"g", 0.2500, 0.7313, 0.0187},
         {"bi", -0.1950, 1.0426, 0.1525}},

        {{"cd", 0.5000, 0.2367, 0.2633},
         {"bi", -0.2020, 0.6923, 0.5097},
         {"and", 1.0000, 0, 0}} },
```

```
{{3.000, 573.79},
        {{"g", 0.2500, 0.7314, 0.0186},
         {"bi", -0.1947, 1.0433, 0.1514},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.2383, 0.2617},
         {"bi", -0.2015, 0.6959, 0.5057},
         {"and", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.3077, 0.0000},
         {"g", 0.2500, 0.7500, 0.0000},
         {"and", 1.0000, 0, 0}} },

{{3.000, 580.00},
        {{"g", 0.2500, 0.7317, 0.0183},
         {"bi", -0.1932, 1.0465, 0.1468},
         {"and", 1.0000, 0, 0}},

        {{"cd", 0.5000, 0.2450, 0.2550},
         {"bi", -0.1999, 0.7108, 0.4890},
         {"and", 1.0000, 0, 0}} }};
```

KF coordinates (zero column to be added)-LEFT

```
phasesubf = {"chl","bi","alm","fst","fctd","and"};

infosubf = {
{{3.000, 480.00},
        {{"chl", 0.1737, 0.8263},
         {"bi", -0.2476, 1.2476}},

        {{"chl", 0.1994, 0.8006},
         {"fctd", 0.5000, 0.5000}},

        {{"fctd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

{{3.000, 491.81},
        {{"fctd", 0.5000, 0.5000},
         {"and", 1.0000, 0}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"chl", 0.1833, 0.8167},
         {"bi", -0.2385, 1.2385}},

        {{"chl", 0.1991, 0.8009},
         {"fctd", 0.5000, 0.5000}} },

{{3.000, 510.52},
        {{"chl", 0.1982, 0.8018},
         {"bi", -0.2213, 1.2213}},

        {{"chl", 0.1988, 0.8012},
         {"fctd", 0.5000, 0.5000}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },
```

```
{{3.000, 511.23},
        {{"chl", 0.1988, 0.8012},
         {"fctd", 0.5000, 0.5000}},

        {{"bi", -0.2206, 1.2206},
         {"fctd", 0.5000, 0.5000}},

        {{"chl", 0.1988, 0.8012},
         {"bi", -0.2206, 1.2206}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 516.50},
        {{"bi", -0.2171, 1.2171},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"bi", -0.2171, 1.2171},
         {"fctd", 0.5000, 0.5000}},

        {{"bi", -0.2171, 1.2171},
         {"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 523.99},
        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"bi", -0.2149, 1.2149},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 524.91},
        {{"bi", -0.2146, 1.2146},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },
```

```
{{3.000, 526.12},
        {{"bi", -0.2142, 1.2142},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 526.96},
        {{"bi", -0.2140, 1.2140},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 534.67},
        {{"bi", -0.2118, 1.2118},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 537.75},
        {{"bi", -0.2109, 1.2109},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 538.50},
        {{"bi", -0.2107, 1.2107},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },

{{3.000, 572.28},
        {{"bi", -0.2013, 1.2013},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}} },
```

```
{{3.000, 573.79},
        {{"fst", 0.6923, 0.3077},
         {"and", 1.0000, 0}},

        {{"alm", 0.2500, 0.7500},
         {"and", 1.0000, 0}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"bi", -0.2009, 1.2009},
         {"alm", 0.2500, 0.7500}} },

{{3.000, 580.00},
        {{"bi", -0.1992, 1.1992},
         {"alm", 0.2500, 0.7500}},

        {{"alm", 0.2500, 0.7500},
         {"and", 1.0000, 0}} }};
```

KM coordinates (zero column to be added) - RIGHT

```
phasesubm = {"chl","bi","py","mst","mctd","and"};

infosubm ={
{{3.000, 480.00},
        {{"bi", -0.3722, 1.3722},
         {"chl", 0.1580, 0.8420}},

        {{"chl", 0.2251, 0.7749},
         {"and", 1.0000, 0}} },

{{3.000, 491.81},
        {{"bi", -0.3700, 1.3700},
         {"chl", 0.1670, 0.8330}},

        {{"chl", 0.2216, 0.7784},
         {"and", 1.0000, 0}} },

{{3.000, 510.52},
        {{"bi", -0.3644, 1.3644},
         {"chl", 0.1810, 0.8190}},

        {{"chl", 0.2163, 0.7837},
         {"and", 1.0000, 0}} },

{{3.000, 511.26},
        {{"bi", -0.3641, 1.3641},
         {"chl", 0.1816, 0.8184}},

        {{"chl", 0.2161, 0.7839},
         {"and", 1.0000, 0}} },

{{3.000, 516.45},
        {{"bi", -0.3622, 1.3622},
         {"chl", 0.1853, 0.8147}},

        {{"chl", 0.2146, 0.7854},
         {"and", 1.0000, 0}} },

{{3.000, 523.98},
        {{"bi", -0.3591, 1.3591},
         {"chl", 0.1907, 0.8093}},

        {{"chl", 0.2126, 0.7874},
         {"and", 1.0000, 0}} },
```

{{3.000, 524.91},
        {{"bi", -0.3587, 1.3587},
         {"chl", 0.1914, 0.8086}},

        {{"chl", 0.2123, 0.7877},
         {"and", 1.0000, 0}} },

{{3.000, 526.12},
        {{"bi", -0.3582, 1.3582},
         {"chl", 0.1923, 0.8077}},

        {{"chl", 0.2120, 0.7880},
         {"and", 1.0000, 0}} },

{{3.000, 526.96},
        {{"chl", 0.2118, 0.7882},
         {"and", 1.0000, 0}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}},

        {{"chl", 0.2118, 0.7882},
         {"cd", 0.5000, 0.5000}},

        {{"bi", -0.3578, 1.3578},
         {"chl", 0.1929, 0.8071}} },

{{3.000, 534.67},
        {{"bi", -0.3543, 1.3543},
         {"chl", 0.1983, 0.8017}},

        {{"chl", 0.2046, 0.7954},
         {"cd", 0.5000, 0.5000}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

{{3.000, 537.75},
        {{"bi", -0.3528, 1.3528},
         {"chl", 0.2008, 0.7992}},

        {{"chl", 0.2018, 0.7982},
         {"cd", 0.5000, 0.5000}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

{{3.000, 538.50},
        {{"bi", -0.3525, 1.3525},
         {"cd", 0.5000, 0.5000}},

        {{"chl", 0.2012, 0.7988},
         {"cd", 0.5000, 0.5000}},

        {{"bi", -0.3525, 1.3525},
         {"chl", 0.2012, 0.7988}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

```
{{3.000, 572.28},
        {{"bi", -0.3482, 1.3482},
         {"cd", 0.5000, 0.5000}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

{{3.000, 573.79},
        {{"bi", -0.3480, 1.3480},
         {"cd", 0.5000, 0.5000}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} },

{{3.000, 580.00},
        {{"bi", -0.3472, 1.3472},
         {"cd", 0.5000, 0.5000}},

        {{"cd", 0.5000, 0.5000},
         {"and", 1.0000, 0}} }};
```

☐ setting up

```
setup["3.0 kbar"];
```

■ plotting

```
make[524.8];
```


AFM
3.0 kbar
524.8

als

st

ctd

g

chl

bi
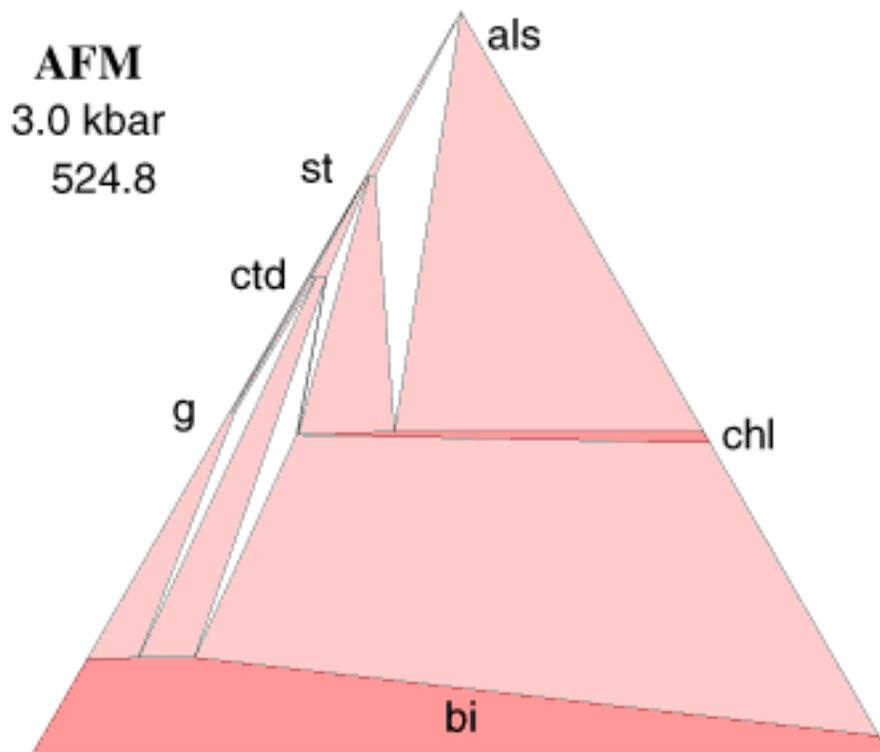
detail around the ctd one-phase field

```
partmake[524.8, {{-0.35,-0.22},{-0.6,-0.45}}];
```

■ AFM compatibility diagrams at 6 kbar

■ AFM system-specific functions

applies function f to AFM coordinates as provided by THERMOCALC,
after converting them into graphical coordinates

```
Clear[conv];
conv[f_,t_]:=(p = Map[(Mg = #[[4]]; Fe = #[[3]];
                      N[ {(Mg - Fe)/Sqrt[3], -(Mg + Fe)} ] )&, t];
              f[Join[p,{p[[1]]}]]);

conv[t_]:= (Mg = t[[4]]; Fe = t[[3]]; N[ {(Mg - Fe)/Sqrt[3], -(Mg + Fe)}]);
```

---

default font sizes

```
fontsize1 = 12; fontsize = 16;

varyTatP = True;
```

---

creates AFM triangle (triangle not joined up, so no bottom line on triangle)

```
third = 1/3;        sqrtthird = 1/Sqrt[3];      twothird = 2/3;

ll = 1.36; lla = ll sqrtthird;
cll = 1 - ll; clla = 1 - cll;
dd = 0.03;

{xky,yky} = {0,0}; xbot = lla + dd sqrtthird; ybot = -ll - dd;

shape = N[{{-xbot,ybot}, {0,0}, {xbot,ybot}}]

{{-0.802517, -1.39}, {0, 0}, {0.802517, -1.39}}
```

---

plot range info

```
xband = 0.191; yband = 0.05;      (* for AspectRatio -> Automatic *)

xlow0 = -xbot - xband; xhigh0 = xbot + xband;
ylow0 = ybot - yband; yhigh0 = yband;

plotrange = {{xlow0,xhigh0},{ylow0,yhigh0}};
plotrangef = plotrange;
```

---

default slider coordinates

```
y = -1.6; dy = 0.02; dy1 = 0.05;
x1 = -0.8; x2 = 0.8;
yplus = 0.032; yminus = -0.075;
```

vscale

```
xsc = -0.77; ysc = -0.32; pl = 1;

plotvscale[v_] := Text[FontForm[N[Round[10^pl v]/10^pl],
                                {"Helvetica",fontsize}], {xsc,ysc},{-1,0}]
```

draws labels

```
Clear[labelling];
labelling[p_] :=
    ({Text[FontForm[p,{"Helvetica",fontsize}], {-0.7,-0.21}],
     Text[FontForm["AFM",{"Times-Bold",18}], {-0.7,-0.1}],
     Text[FontForm["als",{"Helvetica",fontsize}], {0.1,-0.05}],
     Text[FontForm["st",{"Helvetica",fontsize}], {-0.27,-0.3}],
     Text[FontForm["ctd",{"Helvetica",fontsize}], {-0.38,-0.5}],
     Text[FontForm["g",{"Helvetica",fontsize}], {-0.52,-0.75}],
     Text[FontForm["chl",{"Helvetica",fontsize}], {0.54,-0.80}],
     Text[FontForm["bi",{"Helvetica",fontsize}], {0,-1.33}]});
```

assembly of data

```
Clear[assemble];
assemble[tk_] :=
    (infok = interpolatedi[phase, info, tk];
     infosubfk = Map[Map[Insert[#, 0,-1]&, #]&,
                    interpolatedi[phasesubf, infosubf, tk]];
     infosubmk = Map[Map[Insert[#, 0, 3]&, #]&,
                    interpolatedi[phasesubm, infosubm, tk]];
     allinfo = Join[infok,infosubfk,infosubmk]);
```

■ coordinates

□ divariants

KFM coordinates

```
phase = {"chl","bi","g","st","ctd","ky"};

equivalence = {};

info = {
{{6.000, 500.00},
        {{"ctd", 0.5000, 0.3392, 0.1608},
         {"chl", 0.2180, 0.3193, 0.4627},
         {"ky", 1.0000, 0, 0}} },

{{6.000, 509.50},   (* at kfash univariant *)
        {{"st", 0.6923, 0.3077, 0.0000},
         {"ctd", 0.5000, 0.4999, 0.0001},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.3476, 0.1524},
         {"chl", 0.2162, 0.3380, 0.4458},
         {"ky", 1.0000, 0, 0}} },

{{6.000, 521.40},   (* at kfash univariant *)
        {{"ctd", 0.5000, 0.5000, 0.0000},
         {"g", 0.2500, 0.7500, 0.0000},
         {"chl", 0.1847, 0.8151, 0.0002}},

        {{"st", 0.6923, 0.2978, 0.0099},
         {"ctd", 0.5000, 0.4427, 0.0573},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.3579, 0.1421},
         {"chl", 0.2140, 0.3618, 0.4242},
         {"ky", 1.0000, 0, 0}} },

 {{6.000, 526.04},   (* at kfash univariant *)
        {{"g", 0.2500, 0.7500, 0.0000},
         {"chl", 0.1688, 0.8312, 0.0000},
         {"bi", -0.2329, 1.2329, 0.0000}},

        {{"ctd", 0.5000, 0.4917, 0.0083},
         {"g", 0.2500, 0.7451, 0.0049},
         {"chl", 0.1868, 0.7748, 0.0384}},

        {{"st", 0.6923, 0.2936, 0.0141},
         {"ctd", 0.5000, 0.4220, 0.0780},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.3619, 0.1381},
         {"chl", 0.2131, 0.3714, 0.4154},
         {"ky", 1.0000, 0, 0}} },
```

```
{{6.000, 538.03},  (* at kfmash univariant *)
        {{"st", 0.6923, 0.2819, 0.0258},
         {"ctd", 0.5000, 0.3719, 0.1281},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.3722, 0.1278},
         {"chl", 0.2110, 0.3970, 0.3921},
         {"ky", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2821, 0.0256},
         {"ctd", 0.5000, 0.3728, 0.1272},
         {"chl", 0.2109, 0.3982, 0.3909}},

        {{"st", 0.6923, 0.2820, 0.0257},
         {"chl", 0.2109, 0.3970, 0.3920},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.4694, 0.0306},
         {"g", 0.2500, 0.7313, 0.0187},
         {"chl", 0.1921, 0.6806, 0.1274}},

        {{"g", 0.2500, 0.7357, 0.0143},
         {"chl", 0.1767, 0.7208, 0.1025},
         {"bi", -0.2331, 1.0904, 0.1427}} },

 {{6.000, 545.38},
        {{"st", 0.6923, 0.3077, 0.0000},
         {"ctd", 0.5000, 0.5000, 0.0000},
         {"g", 0.2500, 0.7500, 0.0000}},

        {{"st", 0.6923, 0.2888, 0.0189},
         {"ctd", 0.5000, 0.4025, 0.0975},
         {"chl", 0.2054, 0.4703, 0.3242}},

        {{"st", 0.6923, 0.2795, 0.0282},
         {"chl", 0.2096, 0.3825, 0.4079},
         {"ky", 1.0000, 0, 0}},

        {{"ctd", 0.5000, 0.4553, 0.0447},
         {"g", 0.2500, 0.7219, 0.0281},
         {"chl", 0.1951, 0.6291, 0.1758}},

        {{"g", 0.2500, 0.7259, 0.0241},
         {"chl", 0.1815, 0.6611, 0.1574},
         {"bi", -0.2321, 1.0112, 0.2209}} },
```

{{6.000, 554.93},
        {{"st", 0.6923, 0.2959, 0.0118},
         {"g", 0.2500, 0.7086, 0.0414},
         {"chl", 0.1989, 0.5684, 0.2327}},

        {{"st", 0.6923, 0.2959, 0.0118},
         {"ctd", 0.5000, 0.4363, 0.0637},
         {"chl", 0.1989, 0.5684, 0.2327}},

        {{"ctd", 0.5000, 0.4363, 0.0637},
         {"g", 0.2500, 0.7086, 0.0414},
         {"chl", 0.1989, 0.5684, 0.2327}},

        {{"st", 0.6923, 0.2959, 0.0118},
         {"ctd", 0.5000, 0.4363, 0.0637},
         {"g", 0.2500, 0.7086, 0.0414}},

        {{"st", 0.6923, 0.2761, 0.0316},
         {"chl", 0.2080, 0.3648, 0.4272},
         {"ky", 1.0000, 0, 0}},

        {{"g", 0.2500, 0.7121, 0.0379},
         {"chl", 0.1873, 0.5922, 0.2205},
         {"bi", -0.2294, 0.9178, 0.3116}} },

{{6.000, 572.42},
        {{"st", 0.6923, 0.2882, 0.0195},
         {"chl", 0.1976, 0.4845, 0.3178},
         {"bi", -0.2216, 0.7670, 0.4547}},

        {{"st", 0.6923, 0.2882, 0.0195},
         {"g", 0.2500, 0.6831, 0.0669},
         {"bi", -0.2216, 0.7670, 0.4547}},

        {{"g", 0.2500, 0.6831, 0.0669},
         {"chl", 0.1976, 0.4845, 0.3178},
         {"bi", -0.2216, 0.7670, 0.4547}},

        {{"st", 0.6923, 0.2882, 0.0195},
         {"g", 0.2500, 0.6831, 0.0669},
         {"chl", 0.1976, 0.4845, 0.3178}},

        {{"st", 0.6923, 0.2695, 0.0382},
         {"chl", 0.2050, 0.3343, 0.4607},
         {"ky", 1.0000, 0, 0}} },

```
{{6.000, 584.82},
        {{"st", 0.6923, 0.2642, 0.0435},
         {"bi", -0.2203, 0.5119, 0.7084},
         {"ky", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2642, 0.0435},
         {"chl", 0.2030, 0.3140, 0.4830},
         {"ky", 1.0000, 0, 0}},

        {{"chl", 0.2030, 0.3140, 0.4830},
         {"bi", -0.2203, 0.5119, 0.7084},
         {"ky", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2642, 0.0435},
         {"chl", 0.2030, 0.3140, 0.4830},
         {"bi", -0.2203, 0.5119, 0.7084}},

        {{"st", 0.6923, 0.2868, 0.0209},
         {"g", 0.2500, 0.6789, 0.0711},
         {"bi", -0.2178, 0.7537, 0.4641}} },

{{6.000, 591.04},
        {{"st", 0.6923, 0.2860, 0.0217},
         {"g", 0.2500, 0.6766, 0.0734},
         {"bi", -0.2159, 0.7474, 0.4685}},

        {{"st", 0.6923, 0.2650, 0.0427},
         {"bi", -0.2182, 0.5231, 0.6951},
         {"ky", 1.0000, 0, 0}},

        {{"bi", -0.2353, 0.000, 1.2353},
         {"chl", 0.2021, 0.000, 0.7979},
         {"ky", 1.0000, 0.000, 0}} },

{{6.000, 645.06},
        {{"st", 0.6923, 0.2790, 0.0287},
         {"bi", -0.2000, 0.6960, 0.5040},
         {"ky", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2790, 0.0287},
         {"g", 0.2500, 0.6562, 0.0938},
         {"ky", 1.0000, 0, 0}},

        {{"g", 0.2500, 0.6562, 0.0938},
         {"bi", -0.2000, 0.6960, 0.5040},
         {"ky", 1.0000, 0, 0}},

        {{"st", 0.6923, 0.2790, 0.0287},
         {"g", 0.2500, 0.6562, 0.0938},
         {"bi", -0.2000, 0.6960, 0.5040}} },

 {{6.000, 650.00},
        {{"st", 0.6923, 0.3012, 0.0065},
         {"g", 0.2500, 0.7282, 0.0218},
         {"ky", 1.0000, 0, 0}},

        {{"g", 0.2500, 0.6563, 0.0937},
         {"bi", -0.1990, 0.6990, 0.5000},
         {"ky", 1.0000, 0, 0}} }};
```

```
phasesubf = {"chl","bi","alm","fst","fctd","ky"};

infosubf = {
{{6.000, 500.00},
        {{"chl", 0.1477, 0.8523},
         {"bi", -0.2368, 1.2368}},

        {{"chl", 0.1843, 0.8157},
         {"fctd", 0.5000, 0.5000}},

        {{"fctd", 0.5000, 0.5000},
         {"ky", 1.0000, 0}} },

{{6.000, 509.50},
        {{"fctd", 0.5000, 0.5000},
         {"ky", 1.0000, 0}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"chl", 0.1556, 0.8444},
         {"bi", -0.2366, 1.2366}},

        {{"chl", 0.1844, 0.8156},
         {"fctd", 0.5000, 0.5000}} },

{{6.000, 521.40},
        {{"chl", 0.1847, 0.8153},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"chl", 0.1847, 0.8153},
         {"fctd", 0.5000, 0.5000}},

        {{"chl", 0.1652, 0.8348},
         {"bi", -0.2344, 1.2344}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },
```

```
{{6.000, 526.04},
        {{"chl", 0.1688, 0.8312},
         {"alm", 0.2500, 0.7500}},

        {{"bi", -0.2330, 1.2330},
         {"alm", 0.2500, 0.7500}},

        {{"chl", 0.1688, 0.8312},
         {"bi", -0.2330, 1.2330}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}} ,

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 538.03},
        {{"bi", -0.2300, 1.2300},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 545.38},
        {{"fctd", 0.5000, 0.5000},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fctd", 0.5000, 0.5000},
         {"fst", 0.6923, 0.3077}},

        {{"bi", -0.2282, 1.2282},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 554.93},
        {{"bi", -0.2258, 1.2258},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },
```

```
{{6.000, 572.42},
        {{"bi", -0.2217, 1.2217},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 584.82},
        {{"bi", -0.2188, 1.2188},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 591.04},
        {{"bi", -0.2173, 1.2173},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

{{6.000, 645.06},
        {{"bi", -0.2055, 1.2055},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} },

 {{6.000, 650.00},
        {{"bi", -0.2044, 1.2044},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"alm", 0.2500, 0.7500}},

        {{"fst", 0.6923, 0.3077},
         {"ky", 1.0000, 0}} }};
```

KM coordinates (zero column to be added) - RIGHT

```
phasesubm = {"chl","bi","py","mst","mctd","ky"};

infosubm ={
{{6.000, 500.00},
        {{"bi", -0.3074, 1.3074},
         {"chl", 0.1427, 0.8573}},

        {{"chl", 0.2180, 0.7820},
         {"ky", 1.0000, 0}} },

{{6.000, 509.50},
        {{"bi", -0.3033, 1.3033},
         {"chl", 0.1494, 0.8506}},

        {{"chl", 0.2162, 0.7838},
         {"ky", 1.0000, 0}} },

{{6.000, 521.40},
        {{"bi", -0.2964, 1.2964},
         {"chl", 0.1577, 0.8423}},

        {{"chl", 0.2140, 0.7860},
         {"ky", 1.0000, 0}} },

{{6.000, 526.04},
        {{"bi", -0.2933, 1.2933},
         {"chl", 0.1608, 0.8392}},

        {{"chl", 0.2131, 0.7869},
         {"ky", 1.0000, 0}} },

{{6.000, 538.03},
        {{"bi", -0.2846, 1.2846},
         {"chl", 0.1688, 0.8312}},

        {{"chl", 0.2109, 0.7891},
         {"ky", 1.0000, 0}} },

{{6.000, 545.38},
        {{"bi", -0.2787, 1.2787},
         {"chl", 0.1736, 0.8264}},

        {{"chl", 0.2096, 0.7904},
         {"ky", 1.0000, 0}} },

{{6.000, 554.93},
        {{"bi", -0.2705, 1.2705},
         {"chl", 0.1798, 0.8202}},

        {{"chl", 0.2080, 0.7920},
         {"ky", 1.0000, 0}} },

{{6.000, 572.42},
        {{"bi", -0.2541, 1.2541},
         {"chl", 0.1907, 0.8093}},

        {{"chl", 0.2050, 0.7950},
         {"ky", 1.0000, 0}} },
```

```
{{6.000, 584.82},
        {{"bi", -0.2417, 1.2417},
         {"chl", 0.1982, 0.8018}},

        {{"chl", 0.2030, 0.7970},
         {"ky", 1.0000, 0}} },

{{6.000, 591.04},
        {{"bi", -0.2353, 1.2353},
         {"ky", 1.0000, 0}},

        {{"chl", 0.2021, 0.7979},
         {"ky", 1.0000, 0}},

        {{"bi", -0.2353, 1.2353},
         {"chl", 0.2021, 0.7979}} },

{{6.000, 645.06},
        {{"bi", -0.2214, 1.2214},
         {"ky", 1.0000, 0}} },

{{6.000, 650.00},
        {{"bi", -0.2205, 1.2205},
         {"ky", 1.0000, 0}} }};
```

☐ setting up

```
setup["6.0 kbar"];
```

■ plotting

```
make[554.91];
```

AFM
6.0 kbar
554.9

st

ctd

g

als

chl

bi

© bw/rp 1996

```
make[560];
```

AFM
6.0 kbar
560.

st

ctd

g

als

chl

bi

© bw/rp 1996
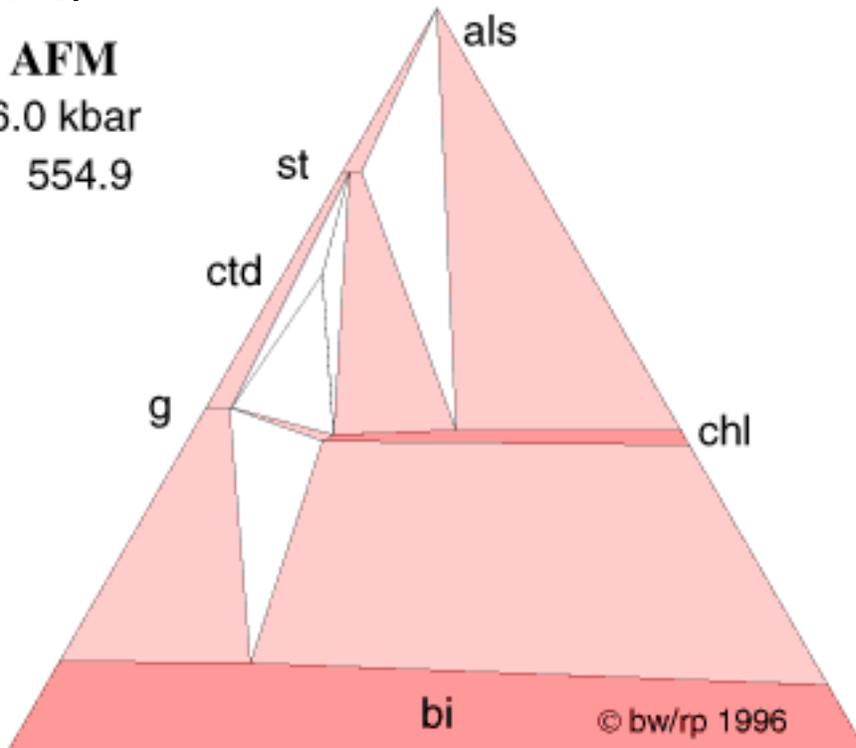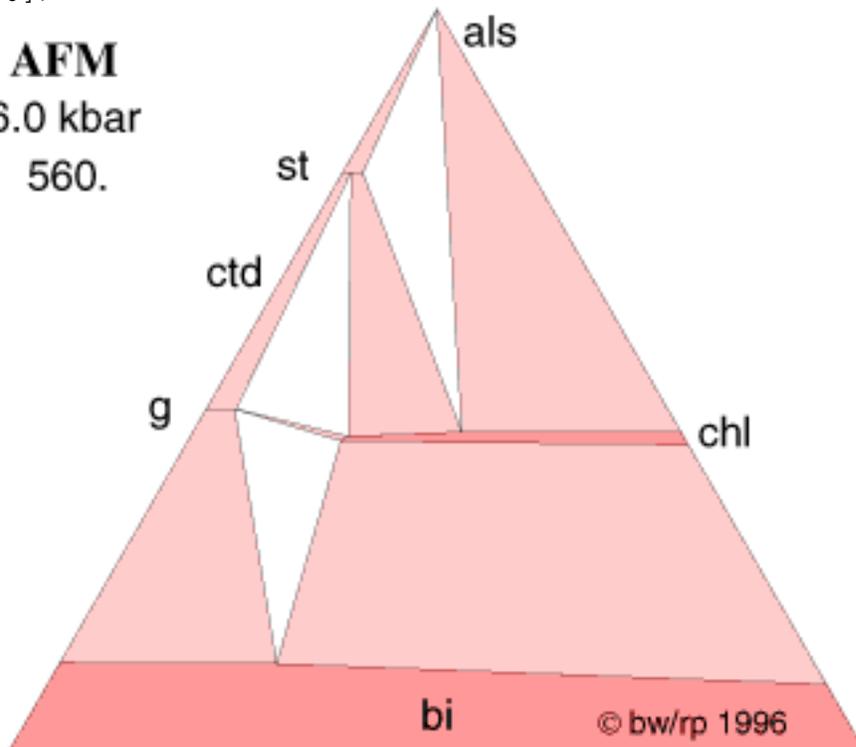
the way to generate a series of diagrams - for animation ...

```
Map[make, Range[555,572,0.5]];
```

■ AFM T-x (range of P)

bulk composition line below garnet - chlorite in AFM

■ definitions

labelling

```
fontsize = 14;  pl = 2;

Clear[labelling];
labelling[ok_] :=
     ({Text[FontForm[ StringJoin["P = ",ToString[N[Round[10^pl ok]/10^pl]]],
                       {"Helvetica",fontsize}], {0.81,632}, {-1,0}],
        Text[FontForm["AFM",{"Times-Bold",22}], {0.852,642}]});
```

───

diagram's (max) coordinates

```
left = 0; right = 1; bottom = 500; top = 650;
```

───

adding

```
addx = 0.05; addy = 0.05;
```

───

T increment in graphics

```
delv = 2;
```

───

it is a T-x diagram

```
varyTatP = True;
```

───

■ data

□ points

```
allpoints = {
{{0,  2,     0, 4.85, 522.5, {"chl"},"g", "bi"},
{0,  2, 0.0265, 5.00, 525.6, {"chl"},"g", "bi"},
{0,  2, 0.0500, 5.14, 528.5, {"chl"},"g", "bi"},
{0,  2, 0.1000, 5.46, 534.8, {"chl"},"g", "bi"},
{0,  2, 0.1500, 5.80, 541.4, {"chl"},"g", "bi"},
{0,  2, 0.1785, 6.00, 545.3, {"chl"},"g", "bi"},
{0,  2, 0.2000, 6.16, 548.3, {"chl"},"g", "bi"},
{0,  2, 0.2500, 6.56, 555.6, {"chl"},"g", "bi"},
{0,  2, 0.3000, 6.98, 563.4, {"chl"},"g", "bi"},
{0,  2, 0.3015, 7.00, 563.6, {"chl"},"g", "bi"},
{0,  2, 0.3500, 7.45, 571.5, {"chl"},"g", "bi"},
{0,  2, 0.4000, 7.95, 580.2, {"chl"},"g", "bi"},
{0,  2, 0.4040, 8.00, 580.9, {"chl"},"g", "bi"},
{0,  2, 0.4500, 8.50, 589.4, {"chl"},"g", "bi"},
{0,  2, 0.4915, 9.00, 597.4, {"chl"},"g", "bi"},
{0,  2, 0.5000, 9.11, 599.1, {"chl"},"g", "bi"},
{0,  2, 0.5500, 9.76, 609.5, {"chl"},"g", "bi"},
{0,  2, 0.5665, 10.00, 613.1, {"chl"},"g", "bi"},
{0,  2, 0.6000, 10.49, 620.6, {"chl"},"g", "bi"},
{0,  2, 0.6325, 11.00, 628.2, {"chl"},"g", "bi"},
{0,  2, 0.6500, 11.28, 632.4, {"chl"},"g", "bi"},
{0,  2, 0.6910, 12.00, 642.8, {"chl"},"g", "bi"},
{0,  2, 0.7000, 12.16, 645.1, {"chl"},"g", "bi"}},

{{0,  2,     0, 7.51, 529.7, {"g"},"chl", "bi"},
{0,  2, 0.0142, 8.00, 537.7, {"g"},"chl", "bi"},
{0,  2, 0.0200, 8.19, 540.7, {"g"},"chl", "bi"},
{0,  2, 0.0400, 8.83, 550.6, {"g"},"chl", "bi"},
{0,  2, 0.0456, 9.00, 553.2, {"g"},"chl", "bi"},
{0,  2, 0.0600, 9.42, 559.6, {"g"},"chl", "bi"},
{0,  2, 0.0800, 9.99, 567.8, {"g"},"chl", "bi"},
{0,  2, 0.0804, 10.00, 568.0, {"g"},"chl", "bi"},
{0,  2, 0.1000, 10.52, 575.4, {"g"},"chl", "bi"},
{0,  2, 0.1186, 11.00, 582.0, {"g"},"chl", "bi"},
{0,  2, 0.1200, 11.03, 582.5, {"g"},"chl", "bi"},
{0,  2, 0.1400, 11.52, 589.1, {"g"},"chl", "bi"},
{0,  2, 0.1600, 11.99, 595.3, {"g"},"chl", "bi"},
{0,  2, 0.1604, 12.00, 595.5, {"g"},"chl", "bi"},
{0,  2, 0.1800, 12.44, 601.2, {"g"},"chl", "bi"},
{0,  2, 0.2000, 12.87, 606.8, {"g"},"chl", "bi"}} };
```

□ univariants

manually reactions.

```
alluni ={
{{1,  1, 5.00, 557.1,  {{"g", "chl"},{"st", "bi"}}},
{1,  1, 6.00, 572.4,  {{"g", "chl"},{"st", "bi"}}},
{1,  1, 7.00, 586.5,  {{"g", "chl"},{"st", "bi"}}},
{1,  1, 8.00, 599.6,  {{"g", "chl"},{"st", "bi"}}},
{1,  1, 9.00, 611.7,  {{"g", "chl"},{"st", "bi"}}},
{1,  1, 9.98, 622.9,  {{"g", "chl"},{"st", "bi"}}}},

{{1,  1, 5.00, 573.3,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 5.25, 576.3,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 5.50, 579.2,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 5.75, 582.0,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 6.00, 584.8,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 6.25, 587.5,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 6.50, 590.2,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 6.75, 592.8,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 7.00, 595.4,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 7.25, 597.9,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 7.50, 600.4,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 7.75, 602.8,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 8.00, 605.2,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 8.25, 607.6,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 8.50, 609.9,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 8.75, 612.1,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 9.00, 614.4,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 9.25, 616.6,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 9.50, 618.8,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 9.75, 620.9,  {{"st", "chl"}, {"bi", "ky"}}},
{1,  1, 9.98, 622.9,  {{"st", "chl"}, {"bi", "ky"}}}},

{{1,  1, 5.00, 624.2,  {{"st", "bi"}, {"g", "sill"}}},
{1,  1, 6.00, 645.1,  {{"st", "bi"}, {"g", "sill"}}},
{1,  1, 7.00, 665.5,  {{"st", "bi"}, {"g", "sill"}}},
{1,  1, 8.00, 685.8,  {{"st", "bi"}, {"g", "sill"}}}},

{{1,  1, 5.00, 676.2,  {{"st", "bi"}, {"g", "ky"}}},
{1,  1, 6.00, 670.0,  {{"st", "bi"}, {"g", "ky"}}},
{1,  1, 7.00, 661.1,  {{"st", "bi"}, {"g", "ky"}}},
{1,  1, 8.00, 650.1,  {{"st", "bi"}, {"g", "ky"}}},
{1,  1, 9.00, 637.2,  {{"st", "bi"}, {"g", "ky"}}},
{1,  1, 9.98, 622.9,  {{"st", "bi"}, {"g", "ky"}}}},

{{1,  1, 9.98, 622.9,   {{"g", "chl"}, {"bi", "ky"}}},
{1,  1, 11.00, 631.3,  {{"g", "chl"}, {"bi", "ky"}}},
{1,  1, 12.00, 638.9,  {{"g", "chl"}, {"bi", "ky"}}}},

{{1,  1, 5.00, 578,  {{"ky"}, {"sill"}}},
{1,  1, 6.00, 623,  {{"ky"}, {"sill"}}},
{1,  1, 7.00, 669,  {{"ky"}, {"sill"}}},
{1,  1, 8.00, 715,  {{"ky"}, {"sill"}}},
{1,  1, 9.00, 762,  {{"ky"}, {"sill"}}},
{1,  1, 10.00, 808,  {{"ky"}, {"sill"}}},
{1,  1, 12.00, 901,  {{"ky"}, {"sill"}}}}    };
```

☐ lines

if two di -> tri boundaries (ie lines) meet at a quadri -> di
(ie a point), then put these in up-temperature (or left->right) order as below

```
alllines = {
{{1,   2, 0,       4.00, 519.1, {"g", "bi"},"chl"},
{1,   2, 0.0500, 4.00, 532.0, {"g", "bi"},"chl"},
{1,   2, 0.1000, 4.00, 544.1, {"g", "bi"},"chl"},
{1,   2, 0.1500, 4.00, 555.7, {"g", "bi"},"chl"},
{1,   2, 0.2000, 4.00, 567.0, {"g", "bi"},"chl"},
{1,   2, 0.2500, 4.00, 578.3, {"g", "bi"},"chl"},
{1,   2, 0.3000, 4.00, 589.5, {"g", "bi"},"chl"},
{1,   2, 0.3500, 4.00, 600.6, {"g", "bi"},"chl"},
{1,   2, 0.4000, 4.00, 611.7, {"g", "bi"},"chl"},

{1,   2, 0,       5.00, 523.0, {"g", "bi"},"chl"},
{1,   2, 0.0500, 5.00, 537.0, {"g", "bi"},"chl"},
{1,   2, 0.1000, 5.00, 549.6, {"g", "bi"},"chl"},
{1,   2, 0.1500, 5.00, 561.6, {"g", "bi"},"chl"},
{1,   2, 0.2000, 5.00, 573.1, {"g", "bi"},"chl"},
{1,   2, 0.2500, 5.00, 584.6, {"g", "bi"},"chl"},
{1,   2, 0.3000, 5.00, 595.9, {"g", "bi"},"chl"},
{1,   2, 0.3500, 5.00, 607.1, {"g", "bi"},"chl"},
{1,   2, 0.4000, 5.00, 618.3, {"g", "bi"},"chl"},

{1,   2, 0,       6.00, 526.0, {"g", "bi"},"chl"},
{1,   2, 0.0500, 6.00, 541.4, {"g", "bi"},"chl"},
{1,   2, 0.1000, 6.00, 554.4, {"g", "bi"},"chl"},
{1,   2, 0.1500, 6.00, 566.6, {"g", "bi"},"chl"},
{1,   2, 0.2000, 6.00, 578.3, {"g", "bi"},"chl"},
{1,   2, 0.2500, 6.00, 589.7, {"g", "bi"},"chl"},
{1,   2, 0.3000, 6.00, 601.1, {"g", "bi"},"chl"},
{1,   2, 0.3500, 6.00, 612.4, {"g", "bi"},"chl"},
{1,   2, 0.4000, 6.00, 623.6, {"g", "bi"},"chl"},

{1,   2, 0.0500, 7.00, 545.5, {"g", "bi"},"chl"},
{1,   2, 0.1000, 7.00, 558.9, {"g", "bi"},"chl"},
{1,   2, 0.1500, 7.00, 571.1, {"g", "bi"},"chl"},
{1,   2, 0.2000, 7.00, 582.8, {"g", "bi"},"chl"},
{1,   2, 0.2500, 7.00, 594.2, {"g", "bi"},"chl"},
{1,   2, 0.3000, 7.00, 605.5, {"g", "bi"},"chl"},
{1,   2, 0.3500, 7.00, 616.7, {"g", "bi"},"chl"},
{1,   2, 0.4000, 7.00, 627.9, {"g", "bi"},"chl"},
{1,   2, 0.4500, 7.00, 639.0, {"g", "bi"},"chl"},

{0,   2, 0,       7.51, 529.7, {"g", "bi"},"chl"},
{1,   2, 0.0500, 7.51, 547.6, {"g", "bi"},"chl"},
{1,   2, 0.1000, 7.51, 561.1, {"g", "bi"},"chl"},
{1,   2, 0.1500, 7.51, 573.3, {"g", "bi"},"chl"},
{1,   2, 0.2000, 7.51, 584.9, {"g", "bi"},"chl"},
{1,   2, 0.2500, 7.51, 596.3, {"g", "bi"},"chl"},
{1,   2, 0.3000, 7.51, 607.5, {"g", "bi"},"chl"},
{1,   2, 0.3500, 7.51, 618.7, {"g", "bi"},"chl"},
{1,   2, 0.4000, 7.51, 629.7, {"g", "bi"},"chl"},
{1,   2, 0.4500, 7.51, 640.8, {"g", "bi"},"chl"},
{1,   2, 0.5000, 7.51, 651.9, {"g", "bi"},"chl"},
```

{0,   2, 0.0142, 8.00, 537.7, {"g", "bi"},"chl"},
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{1,   2, 0.4000, 11.00, 570.0, {"chl"},"g"},
{1,   2, 0.4500, 11.00, 580.8, {"chl"},"g"},
{1,   2, 0.5000, 11.00, 592.5, {"chl"},"g"},
{1,   2, 0.5500, 11.00, 605.1, {"chl"},"g"},
{1,   2, 0.6000, 11.00, 618.7, {"chl"},"g"},
{1,   2, 0.6500, 11.00, 633.5, {"chl"},"g"},
{1,   2, 0.7000, 11.00, 649.4, {"chl"},"g"},
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{1,   2, 0.1000, 12.00, 512.9, {"chl"},"g"},
{1,   2, 0.2000, 12.00, 528.2, {"chl"},"g"},
{1,   2, 0.3000, 12.00, 545.5, {"chl"},"g"},
{1,   2, 0.4000, 12.00, 565.3, {"chl"},"g"},
{1,   2, 0.5000, 12.00, 588.1, {"chl"},"g"},
{1,   2, 0.6000, 12.00, 614.7, {"chl"},"g"},
{1,   2, 0.7000, 12.00, 645.8, {"chl"},"g"},
{1,   2, 0.8000, 12.00, 682.3, {"chl"},"g"}},

(* _____ *)


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{1,   2, 0.1500, 5.00, 524.6, {"chl"},"bi"},
{1,   2, 0.2000, 5.00, 524.0, {"chl"},"bi"},
{1,   2, 0.2500, 5.00, 523.5, {"chl"},"bi"},
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{1,   2,      3, 5.00, 400.0, {"chl"},"bi"},
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{1,   2, 0.1785, 6.00, 545.3, {"chl"},"bi"},      (*****)
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{1,   2,      3, 6.00, 400.0, {"chl"},"bi"},

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{1,   2,      3, 7.00, 400.0, {"chl"},"bi"},
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{1,   2, 0.3000, 9.00, 603.9, {"chl"},"bi"},
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{1,   2, 0.5500, 9.00, 595.1, {"chl"},"bi"},
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{1,   2, 0.3500, 10.00, 622.2, {"chl"},"bi"},
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{1,   2, 0.4500, 10.00, 618.4, {"chl"},"bi"},
{1,   2, 0.5000, 10.00, 616.2, {"chl"},"bi"},
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{1,   2, 0.2000, 11.00, 647.6, {"chl"},"bi"},
{1,   2, 0.2500, 11.00, 645.9, {"chl"},"bi"},
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{1,   2, 0.4500, 11.00, 637.7, {"chl"},"bi"},
{1,   2, 0.5000, 11.00, 635.3, {"chl"},"bi"},
{1,   2, 0.5500, 11.00, 632.8, {"chl"},"bi"},
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{1,   2, 0.6500, 11.00, 627.3, {"chl"},"bi"},
{1,   2, 0.7000, 11.00, 624.2, {"chl"},"bi"},
{1,   2, 0.7500, 11.00, 620.9, {"chl"},"bi"},
{1,   2, 0.8000, 11.00, 617.5, {"chl"},"bi"},
{1,   2, 0.8500, 11.00, 613.9, {"chl"},"bi"},
{1,   2, 0.9000, 11.00, 609.9, {"chl"},"bi"},
{1,   2, 0.9500, 11.00, 605.8, {"chl"},"bi"},
{1,   2, 1.0000, 11.00, 601.3, {"chl"},"bi"},
{1,   2,      3, 11.00, 400.0, {"chl"},"bi"},

{1,   2, 0,        12.00, 675.2, {"chl"},"bi"},
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{1,   2, 0.2000, 12.00, 668.2, {"chl"},"bi"},
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{1,   2, 0.4000, 12.00, 659.5, {"chl"},"bi"},
{1,   2, 0.5000, 12.00, 654.4, {"chl"},"bi"},
{1,   2, 0.6000, 12.00, 648.7, {"chl"},"bi"},
{1,   2, 0.7000, 12.00, 642.2, {"chl"},"bi"},
{1,   2, 0.8000, 12.00, 635.0, {"chl"},"bi"},
{1,   2, 0.9000, 12.00, 626.7, {"chl"},"bi"},
{1,   2, 1.0000, 12.00, 617.4, {"chl"},"bi"},
{1,   2,      3, 12.00, 400.0, {"chl"},"bi"}},  (* manual addition *)
```

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{1,  2, 0.0200, 7.51, 542.9, {"g"},"chl"},
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{1,  2, 0.0400, 7.51, 554.8, {"g"},"chl"},
{1,  2, 0.0500, 7.51, 560.4, {"g"},"chl"},
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{1,  2, 0.0900, 7.51, 580.7, {"g"},"chl"},
{1,  2, 0.1000, 7.51, 585.3, {"g"},"chl"},

{1,  2, 0,        8.00, 528.0, {"g"},"chl"},
{1,  2, 0.0150, 8.00, 538.2, {"g"},"chl"},
{1,  2, 0.0300, 8.00, 547.6, {"g"},"chl"},
{1,  2, 0.0450, 8.00, 556.3, {"g"},"chl"},
{1,  2, 0.0600, 8.00, 564.5, {"g"},"chl"},
{1,  2, 0.0750, 8.00, 572.2, {"g"},"chl"},
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{1,  2, 0.1350, 8.00, 599.4, {"g"},"chl"},
{1,  2, 0.1500, 8.00, 605.5, {"g"},"chl"},

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{1,  2, 0.0450, 9.00, 552.9, {"g"},"chl"},
{1,  2, 0.0500, 9.00, 555.7, {"g"},"chl"},

{1,  2,      0, 10.00, 519.4, {"g"},"chl"},
{1,  2, 0.0200, 10.00, 533.3, {"g"},"chl"},
{1,  2, 0.0400, 10.00, 545.8, {"g"},"chl"},
{1,  2, 0.0600, 10.00, 557.2, {"g"},"chl"},
{1,  2, 0.0800, 10.00, 567.8, {"g"},"chl"},
{1,  2, 0.1000, 10.00, 577.6, {"g"},"chl"},
{1,  2, 0.1200, 10.00, 586.8, {"g"},"chl"},

{1,  2, 0,        11.00, 514.1, {"g"},"chl"},
{1,  2, 0.0120, 11.00, 522.9, {"g"},"chl"},
{1,  2, 0.0240, 11.00, 531.0, {"g"},"chl"},
{1,  2, 0.0360, 11.00, 538.7, {"g"},"chl"},
{1,  2, 0.0480, 11.00, 545.9, {"g"},"chl"},
{1,  2, 0.0600, 11.00, 552.7, {"g"},"chl"},
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{1,  2, 0.1080, 11.00, 577.1, {"g"},"chl"},
{1,  2, 0.1200, 11.00, 582.6, {"g"},"chl"},
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```
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{1,   2, 0.0200, 12.00, 522.9, {"g"},"chl"},
{1,   2, 0.0400, 12.00, 535.9, {"g"},"chl"},
{1,   2, 0.0600, 12.00, 547.7, {"g"},"chl"},
{1,   2, 0.0800, 12.00, 558.5, {"g"},"chl"},
{1,   2, 0.1000, 12.00, 568.6, {"g"},"chl"},
{1,   2, 0.1200, 12.00, 578.0, {"g"},"chl"},
{1,   2, 0.1400, 12.00, 586.9, {"g"},"chl"},
{1,   2, 0.1600, 12.00, 595.3, {"g"},"chl"},
{1,   2, 0.1800, 12.00, 603.3, {"g"},"chl"},
{1,   2, 0.2000, 12.00, 610.9, {"g"},"chl"}},

{{1,   2, 0, 7.51, 400, {"g"},"bi"},
 {1,   2, 0, 7.51, 800, {"g"},"bi"},

 {1,   2, 0.0142, 8, 400, {"g"},"bi"},
 {1,   2, 0.0142, 8, 800, {"g"},"bi"},

 {1,   2, 0.0456, 9, 400, {"g"},"bi"},
 {1,   2, 0.0456, 9, 800, {"g"},"bi"},

 {1,   2, 0.0804, 10, 400, {"g"},"bi"},
 {1,   2, 0.0804, 10, 800, {"g"},"bi"},

 {1,   2, 0.1186, 11, 400, {"g"},"bi"},
 {1,   2, 0.1186, 11, 800, {"g"},"bi"},

 {1,   2, 0.1604, 12, 400, {"g"},"bi"},
 {1,   2, 0.1604, 12, 800, {"g"},"bi"}},

{{1,   2, -1, 7.51, 400, {"g"},"Q"},
 {1,   2, -1, 7.51, 800, {"g"},"Q"},

 {1,   2, -1, 8, 400, {"g"},"Q"},
 {1,   2, -1, 8, 800, {"g"},"Q"},

 {1,   2, -1, 9, 400, {"g"},"Q"},
 {1,   2, -1, 9, 800, {"g"},"Q"},

 {1,   2, -1, 10, 400, {"g"},"Q"},
 {1,   2, -1, 10, 800, {"g"},"Q"},

 {1,   2, -1, 11, 400, {"g"},"Q"},
 {1,   2, -1, 11, 800, {"g"},"Q"},

 {1,   2, -1, 12, 400, {"g"},"Q"},
 {1,   2, -1, 12, 800, {"g"},"Q"}} };
```

☐ assembling data

```
setupvx;
```

■ plotting

```
top = 650; bottom = 510; left = 0; right = 1;
delv = 4;  debugit = False;
makevx[8.5];
```
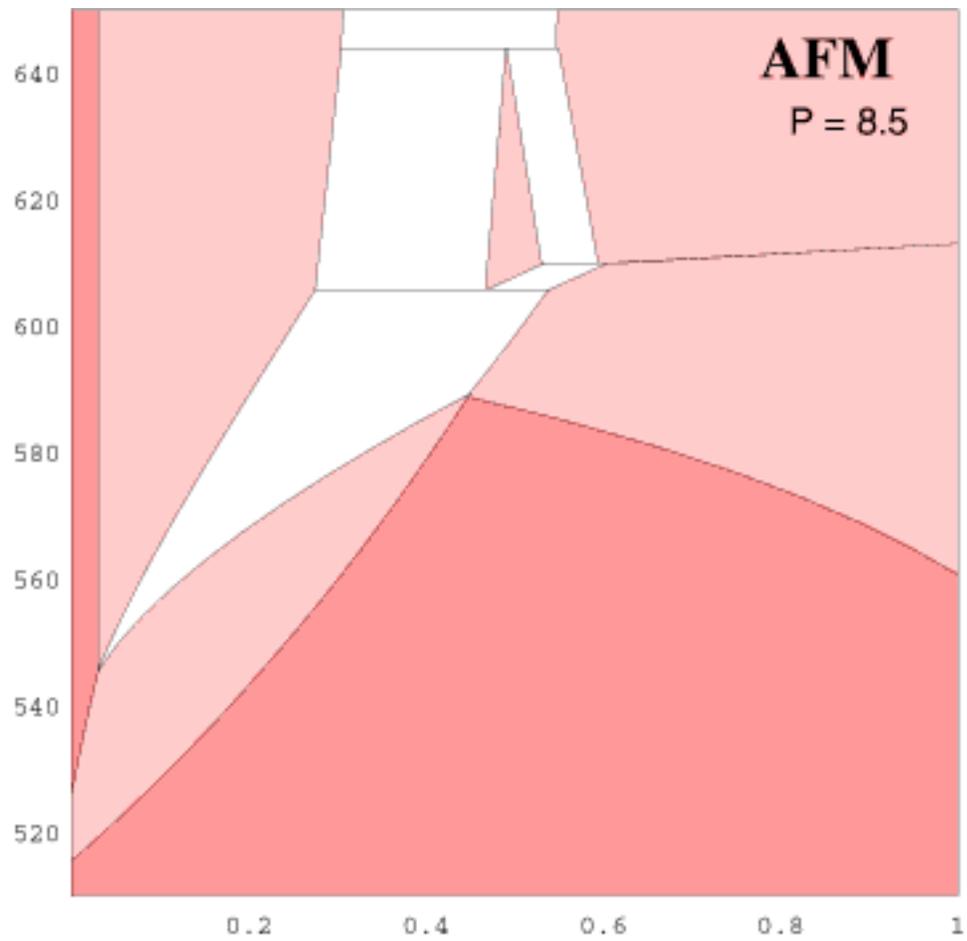

making a series of diagrams for animation

```
Map[makevx, Range[5.0,5.14,0.01]];
```

labelling is tedious:

```
Clear[labelling];
labelling[ok_] :=
    ({Text[FontForm[ StringJoin["P = ",ToString[N[Round[10^pl ok]/10^pl]]],
                    {"Helvetica",fontsize}], {0.81,632}, {-1,0}],
      Text[FontForm["AFM",{"Times-Bold",22}], {0.852,642}],
      Text[FontForm["chl",{"Helvetica",14}], {0.5,520}],
      Text[FontForm["g",{"Helvetica",14}], {0.12,595}],
      Text[FontForm["chl + bi",{"Helvetica",14}], {0.90,608}],
      Text[FontForm["g + bi",{"Helvetica",14}], {0.18,620}],
      Text[FontForm["st + bi",{"Helvetica",14}], {0.78,600}],
      Text[FontForm["ky + bi",{"Helvetica",14}], {0.7,625}],
      Text[FontForm["g + chl",{"Helvetica",14}], {0.18,555}],
      Line[{{0.52,617}, {0.71,600}}],
      Line[{{0.01,590}, {0.1,595}}]}]);

top = 650; bottom = 510; left = 0; right = 1;
delv = 4;  debugit = False;

makevx[8.5];
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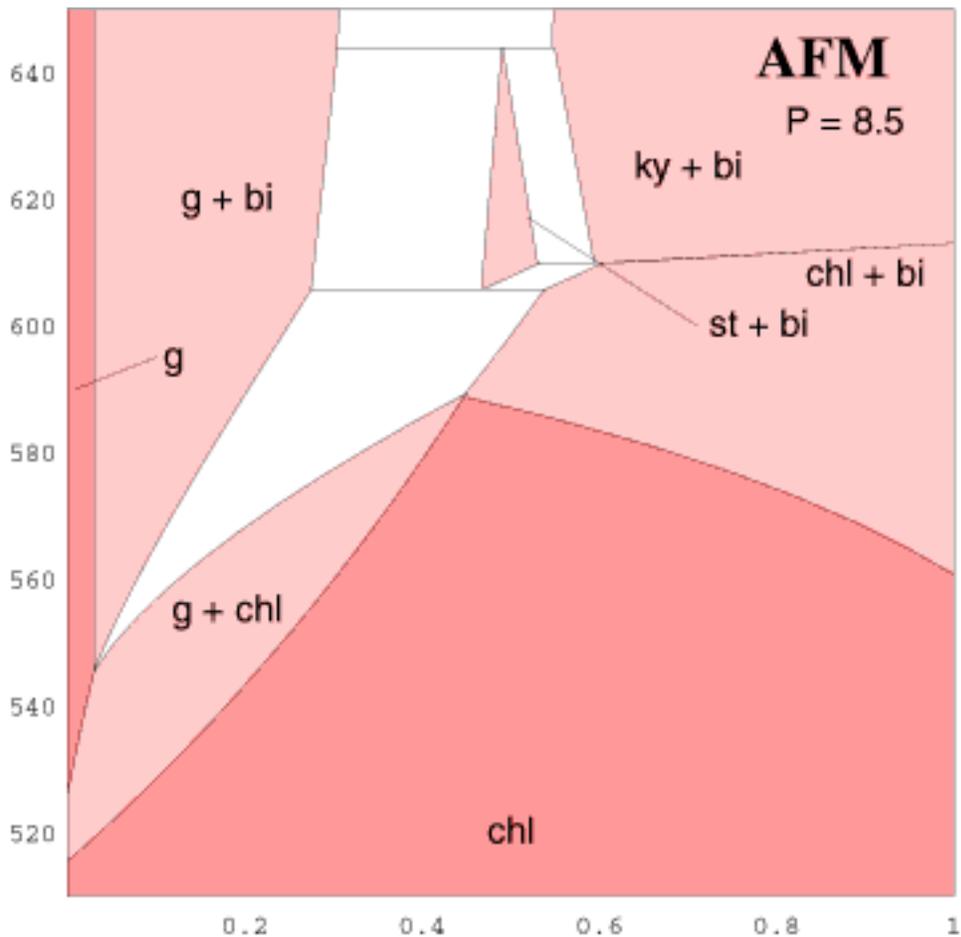
■ AFM P-x at 600°C

bulk composition line below garnet - chlorite in AFM

■ definitions

```
left = 0; right = 1; bottom = 2.0; top = 14.0;
delv = 0.05;

varyTatP = False;
```

■ coordinates

□ points

```
allpoints = {(* corner of g quadri *)
              {{1,  2, 0.1758, 12.34, 600.0, {"g"},"bi", "chl"}},

              (* corner of chl quadri *)
              {{1,  2, 0.5044, 9.16, 600.0, {"chl"},"g", "bi"}}};
```

□ univariants

```
alluni ={
  {{1,  1, 3.55, 600.0,  {{"and"}, {"sill"}}}},
  {{1,  1, 3.88, 600.0,  {{"g", "sill"}, {"st", "bi"}}}},
  {{1,  1, 5.49, 600.0,  {{"sill"}, {"ky"}}}},
  {{1,  1, 7.46, 600.0,  {{"ky", "bi"}, {"st", "chl"}}}},
  {{1,  1, 8.04, 600.0,  {{"st", "bi"}, {"chl", "g"}}}}};
```

□ lines

if two di -> tri boundaries (ie lines) meet at a quadri -> di
(ie a point), then put these in up-temperature (or left->right) order as below

```
alllines = {
{(* cd-and-bi *)
(* bi-and edge *)
{1,  2, 0.0600, 1.77, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.1200, 2.03, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.1800, 2.28, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.2400, 2.53, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.3000, 2.77, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.3600, 3.00, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.4200, 3.23, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.4800, 3.46, 600.0, {"bi", "and"},"cd"},
{1,  2, 0.5400, 3.68, 600.0, {"bi", "and"},"cd"}},

{(* bi-cd edge *)
{1,  2, 0.0600, 1.74, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.1200, 1.98, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.1800, 2.21, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.2400, 2.45, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.3000, 2.68, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.3600, 2.91, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.4200, 3.14, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.4800, 3.36, 600.0, {"cd", "bi"},"and"},
{1,  2, 0.5400, 3.58, 600.0, {"cd", "bi"},"and"}},
```

```
{(* cd-sill-bi *)
(* bi-sill edge *)
{1,   2, 0.4000, 3.24, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.4600, 3.42, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.5200, 3.59, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.5800, 3.76, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.6400, 3.93, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.7000, 4.09, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.7600, 4.25, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.8200, 4.41, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.8800, 4.56, 600.0, {"bi", "sill"},"cd"},
{1,   2, 0.9400, 4.70, 600.0, {"bi", "sill"},"cd"},
{1,   2, 1.0000, 4.85, 600.0, {"bi", "sill"},"cd"}},

{(*bi-cd edge *)
{1,   2, 0.4000, 3.16, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.4600, 3.34, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.5200, 3.52, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.5800, 3.69, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.6400, 3.87, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.7000, 4.04, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.7600, 4.21, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.8200, 4.37, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.8800, 4.53, 600.0, {"cd", "bi"},"sill"},
{1,   2, 0.9400, 4.69, 600.0, {"cd", "bi"},"sill"},
{1,   2, 1.0000, 4.85, 600.0, {"cd", "bi"},"sill"}},

{(* g-and-bi*)
(* g-bi edge *)
{1,   2, 0, 2.29, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0100, 2.42, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0200, 2.54, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0300, 2.67, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0400, 2.81, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0500, 2.94, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0600, 3.07, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0700, 3.21, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0800, 3.35, 600.0, {"g", "bi"},"and"},
{1,   2, 0.0900, 3.49, 600.0, {"g", "bi"},"and"},
{1,   2, 0.1000, 3.63, 600.0, {"g", "bi"},"and"}},

{(* bi-and edge *)
{1,   2, 0, 2.29, 600.0, {"bi", "and"},"g"},
{1,   2, 0.0200, 2.42, 600.0, {"bi", "and"},"g"},
{1,   2, 0.0400, 2.55, 600.0, {"bi", "and"},"g"},
{1,   2, 0.0600, 2.68, 600.0, {"bi", "and"},"g"},
{1,   2, 0.0800, 2.81, 600.0, {"bi", "and"},"g"},
{1,   2, 0.1000, 2.95, 600.0, {"bi", "and"},"g"},
{1,   2, 0.1200, 3.09, 600.0, {"bi", "and"},"g"},
{1,   2, 0.1400, 3.23, 600.0, {"bi", "and"},"g"},
{1,   2, 0.1600, 3.37, 600.0, {"bi", "and"},"g"},
{1,   2, 0.1800, 3.52, 600.0, {"bi", "and"},"g"},
{1,   2, 0.2000, 3.67, 600.0, {"bi", "and"},"g"}},
```

```
{(* g-sill-bi *)
(* g-bi edge *)
{1,   2, 0.0500, 2.87, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.0600, 3.02, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.0700, 3.17, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.0800, 3.33, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.0900, 3.48, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1000, 3.64, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1100, 3.80, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1200, 3.96, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1300, 4.13, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1400, 4.30, 600.0, {"g",  "bi"},"sill"},
{1,   2, 0.1500, 4.47, 600.0, {"g",  "bi"},"sill"}},

{(* bi-sill edge *)
{1,   2, 0.1500, 3.27, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.1600, 3.35, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.1700, 3.44, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.1800, 3.52, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.1900, 3.60, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2000, 3.69, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2100, 3.77, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2200, 3.86, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2300, 3.94, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2400, 4.03, 600.0, {"bi",  "sill"},"g"},
{1,   2, 0.2500, 4.12, 600.0, {"bi",  "sill"},"g"}},

{(* st-g-bi *)
(* g-bi edge *)
{1,   2, 0.0300, 1.93, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.0900, 3.28, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.1200, 4.01, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.1500, 4.79, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.1800, 5.62, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.2100, 6.52, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.2400, 7.47, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.2700, 8.48, 600.0, {"g",  "bi"},"st"},
{1,   2, 0.3000, 9.54, 600.0, {"g",  "bi"},"st"}},

{(* st-bi edge *)
{1,   2, 0.1000, 2.56, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.1800, 3.62, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.2200, 4.19, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.2600, 4.79, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.3000, 5.42, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.3400, 6.09, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.3800, 6.80, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.4200, 7.57, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.4600, 8.40, 600.0, {"st",  "bi"},"g"},
{1,   2, 0.5000, 9.30, 600.0, {"st",  "bi"},"g"}},

{(* st-sill-bi *)
(* st-bi edge *)
{1,   2, 0.1000, 3.44, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.1500, 3.66, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.2000, 3.88, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.2500, 4.13, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.3000, 4.40, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.3500, 4.68, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.4000, 4.99, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.4500, 5.33, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.5000, 5.69, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.5500, 6.09, 600.0, {"st",  "bi"},"sill"},
{1,   2, 0.6000, 6.53, 600.0, {"st",  "bi"},"sill"}},
```

```
{(* bi-sill edge *)
{1,   2, 0.1000, 3.40, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.1500, 3.58, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.2000, 3.78, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.2500, 4.00, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.3000, 4.22, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.3500, 4.47, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.4000, 4.73, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.4500, 5.01, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.5000, 5.32, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.5500, 5.66, 600.0, {"bi",  "sill"},"st"},
{1,   2, 0.6000, 6.02, 600.0, {"bi",  "sill"},"st"}},

{(* st-ky-bi *)
(* st-bi edge *)
{1,   2, 0.4500, 4.80, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.4600, 5.09, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.4700, 5.41, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.4800, 5.74, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.4900, 6.10, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5000, 6.49, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5100, 6.91, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5200, 7.36, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5300, 7.86, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5400, 8.40, 600.0, {"st",  "bi"},"ky"},
{1,   2, 0.5500, 9.00, 600.0, {"st",  "bi"},"ky"}},

{(* bi-ky edge *)
{1,   2, 0.5000, 4.82, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5100, 5.07, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5200, 5.34, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5300, 5.63, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5400, 5.93, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5500, 6.25, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5600, 6.59, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5700, 6.96, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5800, 7.34, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.5900, 7.76, 600.0, {"bi",  "ky"},"st"},
{1,   2, 0.6000, 8.21, 600.0, {"bi",  "ky"},"st"}},

{(* ky-bi-chl *)
(* bi-ky edge *)
{1,   2, 0.5000, 7.56, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.5500, 7.50, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.6000, 7.44, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.6500, 7.38, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.7000, 7.32, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.7500, 7.26, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.8000, 7.19, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.8500, 7.13, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.9000, 7.07, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 0.9500, 7.00, 600.0, {"bi",  "ky"},"chl"},
{1,   2, 1.0000, 6.94, 600.0, {"bi",  "ky"},"chl"}},

{(* bi-chl edge *)
{1,   2, 0.5000, 7.58, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.5500, 7.52, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.6000, 7.46, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.6500, 7.40, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.7500, 7.27, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.8000, 7.21, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.8500, 7.14, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.9000, 7.07, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 0.9500, 7.01, 600.0, {"chl",  "bi"},"ky"},
{1,   2, 1.0000, 6.94, 600.0, {"chl",  "bi"},"ky"}},
```

```
{(* st-bi-chl *)
(* st-bi edge *)
{1,   2, 0.4000, 8.32, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.4200, 8.19, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.4400, 8.05, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.4600, 7.91, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.4800, 7.77, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.5000, 7.63, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.5200, 7.48, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.5400, 7.32, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.5600, 7.17, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.5800, 7.01, 600.0, {"st",  "bi"},"chl"},
{1,   2, 0.6000, 6.85, 600.0, {"st",  "bi"},"chl"}},

{(* bi-chl edge *)
{1,   2, 0.4000, 8.69, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.4200, 8.58, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.4400, 8.47, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.4600, 8.36, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.4800, 8.24, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.5000, 8.11, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.5200, 7.99, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.5400, 7.86, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.5600, 7.72, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.5800, 7.58, 600.0, {"chl",  "bi"},"st"},
{1,   2, 0.6000, 7.44, 600.0, {"chl",  "bi"},"st"}},

{(* g-bi-chl *)
(* g-bi edge *)
{1,   2, 0.1758, 12.34, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.1800, 12.16, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.2000, 11.21, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.2200, 10.16, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.2400, 9.02, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.2600, 7.86, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.2800, 6.76, 600.0, {"g",  "bi"},"chl"},
{1,   2, 0.3000, 5.78, 600.0, {"g",  "bi"},"chl"}},

{(* bi-chl edge *)
{1,   2, 0.5044, 9.16, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5045, 9.14, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5050, 9.07, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5055, 9.00, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5060, 8.92, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5065, 8.85, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5070, 8.78, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5075, 8.71, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5080, 8.64, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5085, 8.57, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5090, 8.49, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5095, 8.42, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5100, 8.35, 600.0, {"chl",  "bi"},"g"},
{1,   2, 0.5200, 7.08, 600.0, {"chl",  "bi"},"g"}},

{(* g-chl edge *)
{1,   2, 0.1758, 12.34, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.1900, 12.17, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.2300, 11.71, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.3100, 10.85, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.3500, 10.46, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.3900, 10.09, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.4300, 9.75, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.4700, 9.42, 600.0, {"g",  "chl"},"bi"},
{1,   2, 0.5044, 9.16, 600.0, {"g",  "chl"},"bi"}}};
```

```
allqlines = {
{(* g *)
(* g-bi *)
{1,   2, 0, 7.68, 600.0, {"g"},"bi"},
{1,   2, 0.0200, 8.28, 600.0, {"g"},"bi"},
{1,   2, 0.0400, 8.86, 600.0, {"g"},"bi"},
{1,   2, 0.0600, 9.42, 600.0, {"g"},"bi"},
{1,   2, 0.0800, 9.96, 600.0, {"g"},"bi"},
{1,   2, 0.1000, 10.49, 600.0, {"g"},"bi"},
{1,   2, 0.1200, 11.00, 600.0, {"g"},"bi"},
{1,   2, 0.1400, 11.50, 600.0, {"g"},"bi"},
{1,   2, 0.1600, 11.98, 600.0, {"g"},"bi"},
{1,   2, 0.1800, 12.44, 600.0, {"g"},"bi"},
{1,   2, 0.2000, 12.89, 600.0, {"g"},"bi"}},

{(* g-chl *)
{1,   2, 0.1400, 8.59, 600.0, {"g"},"chl"},
{1,   2, 0.1600, 10.93, 600.0, {"g"},"chl"},
{1,   2, 0.1800, 12.69, 600.0, {"g"},"chl"},
{1,   2, 0.2000, 14.18, 600.0, {"g"},"chl"}},

{(* g-q *)             (* manually entered boundary to make quadri work *)
{1,   2, -1, 5.0, 600.0, {"g"},"q"},
{1,   2, -1, 14.0, 600.0, {"g"},"q"}},

{(* chl *)
(* chl-bi *)
{1,   2, 0.4800, 9.11, 600.0, {"chl"},"bi"},
{1,   2, 0.5000, 9.15, 600.0, {"chl"},"bi"},
{1,   2, 0.5200, 9.19, 600.0, {"chl"},"bi"},
{1,   2, 0.5400, 9.24, 600.0, {"chl"},"bi"},
{1,   2, 0.5600, 9.28, 600.0, {"chl"},"bi"},
{1,   2, 0.5800, 9.33, 600.0, {"chl"},"bi"},
{1,   2, 0.6000, 9.38, 600.0, {"chl"},"bi"},
{1,   2, 0.6200, 9.43, 600.0, {"chl"},"bi"},
{1,   2, 0.6400, 9.48, 600.0, {"chl"},"bi"},
{1,   2, 0.6600, 9.54, 600.0, {"chl"},"bi"},
{1,   2, 0.6800, 9.60, 600.0, {"chl"},"bi"},
{1,   2, 0.7000, 9.66, 600.0, {"chl"},"bi"},
{1,   2, 0.7200, 9.72, 600.0, {"chl"},"bi"},
{1,   2, 0.7400, 9.78, 600.0, {"chl"},"bi"},
{1,   2, 0.7600, 9.85, 600.0, {"chl"},"bi"},
{1,   2, 0.7800, 9.92, 600.0, {"chl"},"bi"},
{1,   2, 0.8000, 9.99, 600.0, {"chl"},"bi"},
{1,   2, 0.8200, 10.07, 600.0, {"chl"},"bi"},
{1,   2, 0.8400, 10.15, 600.0, {"chl"},"bi"},
{1,   2, 0.8600, 10.23, 600.0, {"chl"},"bi"},
{1,   2, 0.8800, 10.32, 600.0, {"chl"},"bi"},
{1,   2, 0.9000, 10.41, 600.0, {"chl"},"bi"},
{1,   2, 0.9200, 10.50, 600.0, {"chl"},"bi"},
{1,   2, 0.9400, 10.60, 600.0, {"chl"},"bi"},
{1,   2, 0.9600, 10.70, 600.0, {"chl"},"bi"},
{1,   2, 0.9800, 10.81, 600.0, {"chl"},"bi"},
{1,   2, 1.0000, 10.92, 600.0, {"chl"},"bi"}},

{(* chl-g edge *)
{1,   2, 0.5000, 8.77, 600.0, {"chl"},"g"},
{1,   2, 0.5200, 10.34, 600.0, {"chl"},"g"},
{1,   2, 0.5400, 11.61, 600.0, {"chl"},"g"},
{1,   2, 0.5600, 12.76, 600.0, {"chl"},"g"},
{1,   2, 0.5800, 13.84, 600.0, {"chl"},"g"},
{1,   2, 0.6000, 14.88, 600.0, {"chl"},"g"}},
```

```
{(* chl-q *)      (* manually entered boundary to make quadri work *)
{1,   2, 2, 11.0, 600.0, {"chl"},"q"},
{1,   2, 2, 14.0, 600.0, {"chl"},"q"}}};
```

☐ assembling data

```
setupvx;
```

■ plotting

```
bottom = 2; top = 14; left = 0; right = 1;
delv = 0.05;
makevx[600];
```

AFM
(+ mu + q + H$_2$O)   600°C

P (kbar)

g

g chl

chl

g bi

chl bi

bi sill

bi st

bi ky

bi and

bi cd

Mg/Mg+Fe
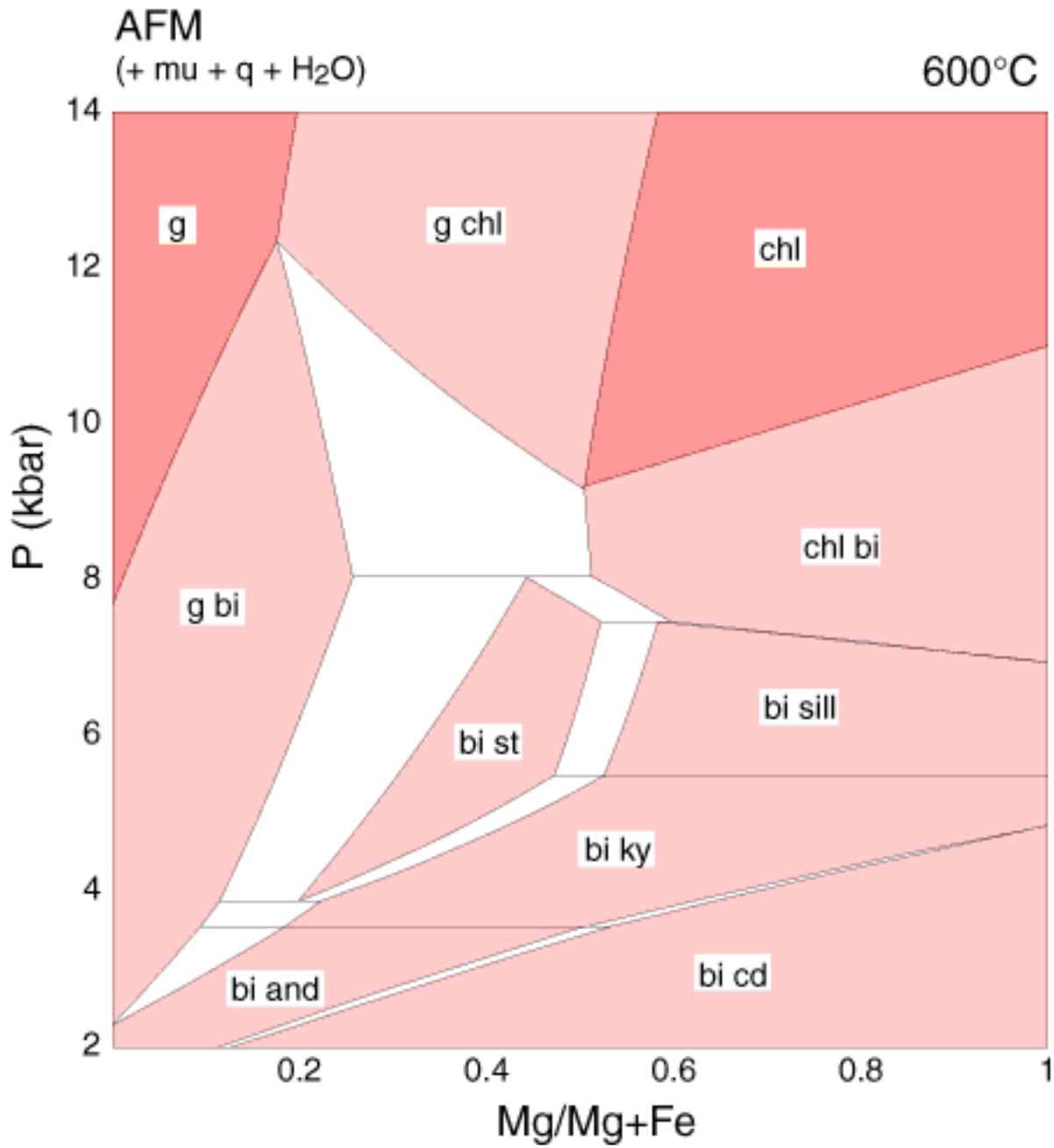
AFM T-y at 6 kbars

bulk composition line through aluminosilicate at x = 0.6

■ definitions

```
varyTatP = True;

left = 0; right = 1; bottom = 500; top = 650;
delv = 2; addx = 0; addy = 0;

fontsize = 14;  pl = 2;

Clear[labelling];
labelling[ok_] :=
     ({Text[FontForm[ StringJoin["P = ",ToString[N[Round[10^pl ok]/10^pl]]],
                      {"Helvetica",fontsize}], {0.01,635}, {-1,0}],
       Text[FontForm["AFM",{"Times-Bold",22}], {0.01,642}, {-1,0}]});
```

■ coordinates

□ points

```
allpoints = {

(* bi *)


{{1,   2, 0.1460, 6.00, 574.5, {"bi"},"st", "chl"}},
{{1,   2, 0.1590, 6.00, 628.2, {"bi"},"st", "g"}},

(* chl *)


{{1,   2, 0.4370, 6.00, 544.8, {"chl"},"st", "ctd"}},
{{1,   2, 0.4230, 6.00, 573.5, {"chl"},"st", "bi"}},

(* ky *)


{{1,   2, 0.9630, 6.00, 585.5, {"ky"},"chl", "bi"}}};
```

□ univariants

```
alluni ={
 {{1,  1, 6.00, 537.9,  {{"ctd", "ky"},{"st", "chl"}}}},
 {{1,  1, 6.00, 584.8,  {{"st", "chl"}, {"bi", "ky"}}}},
 {{1,  1, 6.00, 645.1,  {{"st", "bi"}, {"g", "sill"}}}},
 {{1,  1, 6.00, 623.4,  {{"ky"}, {"sill"}}}}};
```

□ lines

```
alllines = {
(* ky-ctd-chl *)
{(* ctd-chl edge *)
{1,  2, 0.5200, 6.00, 543.8, {"ctd", "chl"},"ky"},
{1,  2, 0.5400, 6.00, 536.0, {"ctd", "chl"},"ky"},
{1,  2, 0.5600, 6.00, 526.8, {"ctd", "chl"},"ky"},
{1,  2, 0.5800, 6.00, 516.1, {"ctd", "chl"},"ky"},
{1,  2, 0.6000, 6.00, 503.6, {"ctd", "chl"},"ky"},
{1,  2, 0.6060, 6.00, 499.5, {"ctd", "chl"},"ky"}},

{(* ky-chl edge *)
{1,  2, 0.9200, 6.00, 538.1, {"chl", "ky"},"ctd"},
{1,  2, 0.9225, 6.00, 537.2, {"chl", "ky"},"ctd"},
{1,  2, 0.9250, 6.00, 536.1, {"chl", "ky"},"ctd"},
{1,  2, 0.9275, 6.00, 535.0, {"chl", "ky"},"ctd"},
{1,  2, 0.9300, 6.00, 533.8, {"chl", "ky"},"ctd"},
{1,  2, 0.9325, 6.00, 532.6, {"chl", "ky"},"ctd"},
{1,  2, 0.9350, 6.00, 531.3, {"chl", "ky"},"ctd"},
{1,  2, 0.9375, 6.00, 529.8, {"chl", "ky"},"ctd"},
{1,  2, 0.9400, 6.00, 528.3, {"chl", "ky"},"ctd"},
{1,  2, 0.9425, 6.00, 526.7, {"chl", "ky"},"ctd"},
{1,  2, 0.9450, 6.00, 525.0, {"chl", "ky"},"ctd"},
{1,  2, 0.9475, 6.00, 523.2, {"chl", "ky"},"ctd"},
{1,  2, 0.9500, 6.00, 521.2, {"chl", "ky"},"ctd"},
{1,  2, 0.9525, 6.00, 519.1, {"chl", "ky"},"ctd"},
{1,  2, 0.9550, 6.00, 516.7, {"chl", "ky"},"ctd"},
{1,  2, 0.9575, 6.00, 514.2, {"chl", "ky"},"ctd"},
{1,  2, 0.9600, 6.00, 511.5, {"chl", "ky"},"ctd"},
{1,  2, 0.9625, 6.00, 508.5, {"chl", "ky"},"ctd"},
{1,  2, 0.9650, 6.00, 505.3, {"chl", "ky"},"ctd"},
{1,  2, 0.9675, 6.00, 501.7, {"chl", "ky"},"ctd"},
{1,  2, 0.9700, 6.00, 497.8, {"chl", "ky"},"ctd"}},

(* st-ctd-chl *)
{(* ctd-chl edge *)
{1,  2, 0.4370, 6.00, 544.8, {"ctd", "chl"},"st"},
{1,  2, 0.4400, 6.00, 544.6, {"ctd", "chl"},"st"},
{1,  2, 0.4600, 6.00, 543.5, {"ctd", "chl"},"st"},
{1,  2, 0.4800, 6.00, 542.3, {"ctd", "chl"},"st"},
{1,  2, 0.5000, 6.00, 540.9, {"ctd", "chl"},"st"},
{1,  2, 0.5200, 6.00, 539.3, {"ctd", "chl"},"st"},
{1,  2, 0.5400, 6.00, 537.5, {"ctd", "chl"},"st"}},

{(* st-chl edge *)
{1,  2, 0.4370, 6.00, 544.8, {"st", "chl"},"ctd"},
{1,  2, 0.4400, 6.00, 544.7, {"st", "chl"},"ctd"},
{1,  2, 0.4600, 6.00, 544.0, {"st", "chl"},"ctd"},
{1,  2, 0.4800, 6.00, 543.2, {"st", "chl"},"ctd"},
{1,  2, 0.5000, 6.00, 542.3, {"st", "chl"},"ctd"},
{1,  2, 0.5200, 6.00, 541.3, {"st", "chl"},"ctd"},
{1,  2, 0.5400, 6.00, 540.2, {"st", "chl"},"ctd"},
{1,  2, 0.5600, 6.00, 538.9, {"st", "chl"},"ctd"},
{1,  2, 0.5800, 6.00, 537.4, {"st", "chl"},"ctd"}},
```

```
(* ky-st-chl *)
{(* st-chl edge *)
{1,   2, 0.5600, 6.00, 533.0, {"st", "chl"},"ky"},
{1,   2, 0.5800, 6.00, 540.8, {"st", "chl"},"ky"},
{1,   2, 0.6000, 6.00, 550.3, {"st", "chl"},"ky"},
{1,   2, 0.6200, 6.00, 562.1, {"st", "chl"},"ky"},
{1,   2, 0.6400, 6.00, 576.7, {"st", "chl"},"ky"},
{1,   2, 0.6600, 6.00, 594.8, {"st", "chl"},"ky"}},

{(* ky-chl edge *)
{1,   2, 0.9200, 6.00, 537.6, {"chl", "ky"},"st"},
{1,   2, 0.9225, 6.00, 539.1, {"chl", "ky"},"st"},
{1,   2, 0.9250, 6.00, 540.8, {"chl", "ky"},"st"},
{1,   2, 0.9275, 6.00, 542.6, {"chl", "ky"},"st"},
{1,   2, 0.9300, 6.00, 544.6, {"chl", "ky"},"st"},
{1,   2, 0.9325, 6.00, 546.8, {"chl", "ky"},"st"},
{1,   2, 0.9350, 6.00, 549.3, {"chl", "ky"},"st"},
{1,   2, 0.9375, 6.00, 552.1, {"chl", "ky"},"st"},
{1,   2, 0.9400, 6.00, 555.3, {"chl", "ky"},"st"},
{1,   2, 0.9425, 6.00, 559.0, {"chl", "ky"},"st"},
{1,   2, 0.9450, 6.00, 563.1, {"chl", "ky"},"st"},
{1,   2, 0.9475, 6.00, 568.0, {"chl", "ky"},"st"},
{1,   2, 0.9500, 6.00, 573.5, {"chl", "ky"},"st"},
{1,   2, 0.9525, 6.00, 580.2, {"chl", "ky"},"st"},
{1,   2, 0.9550, 6.00, 588.0, {"chl", "ky"},"st"}},

(* st-bi-chl *)
{(* st-chl edge *)
{1,   2, 0.4230, 6.00, 573.5, {"st", "chl"},"bi"},
{1,   2, 0.4400, 6.00, 573.9, {"st", "chl"},"bi"},
{1,   2, 0.4600, 6.00, 574.4, {"st", "chl"},"bi"},
{1,   2, 0.4800, 6.00, 574.9, {"st", "chl"},"bi"},
{1,   2, 0.5000, 6.00, 575.6, {"st", "chl"},"bi"},
{1,   2, 0.5200, 6.00, 576.3, {"st", "chl"},"bi"},
{1,   2, 0.5400, 6.00, 577.1, {"st", "chl"},"bi"},
{1,   2, 0.5600, 6.00, 578.0, {"st", "chl"},"bi"},
{1,   2, 0.5800, 6.00, 579.1, {"st", "chl"},"bi"},
{1,   2, 0.6000, 6.00, 580.4, {"st", "chl"},"bi"},
{1,   2, 0.6200, 6.00, 582.0, {"st", "chl"},"bi"},
{1,   2, 0.6400, 6.00, 583.8, {"st", "chl"},"bi"},
{1,   2, 0.6600, 6.00, 586.0, {"st", "chl"},"bi"},
{1,   2, 0.6800, 6.00, 588.7, {"st", "chl"},"bi"},
{1,   2, 0.7000, 6.00, 591.8, {"st", "chl"},"bi"}},
```

```
{(* st-bi edge *)
{1,  2, 0.1460, 6.00, 574.5, {"st", "bi"},"chl"},
{1,  2, 0.1600, 6.00, 574.6, {"st", "bi"},"chl"},
{1,  2, 0.1800, 6.00, 574.8, {"st", "bi"},"chl"},
{1,  2, 0.2000, 6.00, 574.9, {"st", "bi"},"chl"},
{1,  2, 0.2200, 6.00, 575.1, {"st", "bi"},"chl"},
{1,  2, 0.2400, 6.00, 575.3, {"st", "bi"},"chl"},
{1,  2, 0.2600, 6.00, 575.6, {"st", "bi"},"chl"},
{1,  2, 0.2800, 6.00, 575.8, {"st", "bi"},"chl"},
{1,  2, 0.3000, 6.00, 576.1, {"st", "bi"},"chl"},
{1,  2, 0.3200, 6.00, 576.3, {"st", "bi"},"chl"},
{1,  2, 0.3400, 6.00, 576.6, {"st", "bi"},"chl"},
{1,  2, 0.3600, 6.00, 577.0, {"st", "bi"},"chl"},
{1,  2, 0.3800, 6.00, 577.3, {"st", "bi"},"chl"},
{1,  2, 0.4000, 6.00, 577.7, {"st", "bi"},"chl"},
{1,  2, 0.4200, 6.00, 578.2, {"st", "bi"},"chl"},
{1,  2, 0.4400, 6.00, 578.6, {"st", "bi"},"chl"},
{1,  2, 0.4600, 6.00, 579.2, {"st", "bi"},"chl"},
{1,  2, 0.4800, 6.00, 579.7, {"st", "bi"},"chl"},
{1,  2, 0.5000, 6.00, 580.4, {"st", "bi"},"chl"},
{1,  2, 0.5200, 6.00, 581.1, {"st", "bi"},"chl"},
{1,  2, 0.5400, 6.00, 582.0, {"st", "bi"},"chl"},
{1,  2, 0.5600, 6.00, 582.9, {"st", "bi"},"chl"},
{1,  2, 0.5800, 6.00, 584.0, {"st", "bi"},"chl"},
{1,  2, 0.6000, 6.00, 585.3, {"st", "bi"},"chl"},
{1,  2, 0.6200, 6.00, 586.7, {"st", "bi"},"chl"},
{1,  2, 0.6400, 6.00, 588.4, {"st", "bi"},"chl"},
{1,  2, 0.6600, 6.00, 590.3, {"st", "bi"},"chl"}},

{(* bi-chl edge *)
{1,  2, 0.1460, 6.00, 574.5, {"chl", "bi"},"st"},
{1,  2, 0.1600, 6.00, 574.4, {"chl", "bi"},"st"},
{1,  2, 0.2000, 6.00, 574.3, {"chl", "bi"},"st"},
{1,  2, 0.2400, 6.00, 574.2, {"chl", "bi"},"st"},
{1,  2, 0.2800, 6.00, 574.1, {"chl", "bi"},"st"},
{1,  2, 0.3000, 6.00, 574.0, {"chl", "bi"},"st"},
{1,  2, 0.3400, 6.00, 573.9, {"chl", "bi"},"st"},
{1,  2, 0.3600, 6.00, 573.8, {"chl", "bi"},"st"},
{1,  2, 0.3800, 6.00, 573.7, {"chl", "bi"},"st"},
{1,  2, 0.4000, 6.00, 573.6, {"chl", "bi"},"st"},
{1,  2, 0.4225, 6.00, 573.5, {"chl", "bi"},"st"}},

(* ky-st-bi *)
{(* st-bi edge *)
{1,  2, 0.5000, 6.00, 630.5, {"st", "bi"},"ky"},
{1,  2, 0.5200, 6.00, 623.2, {"st", "bi"},"ky"},
{1,  2, 0.5400, 6.00, 614.8, {"st", "bi"},"ky"},
{1,  2, 0.5600, 6.00, 605.1, {"st", "bi"},"ky"},
{1,  2, 0.5800, 6.00, 593.6, {"st", "bi"},"ky"},
{1,  2, 0.6000, 6.00, 579.8, {"st", "bi"},"ky"}},

{(* ky-bi edge *)
{1,  2, 0.9200, 6.00, 632.0, {"bi", "ky"},"st"},
{1,  2, 0.9300, 6.00, 622.7, {"bi", "ky"},"st"},
{1,  2, 0.9400, 6.00, 609.9, {"bi", "ky"},"st"},
{1,  2, 0.9500, 6.00, 591.5, {"bi", "ky"},"st"},
{1,  2, 0.9600, 6.00, 563.7, {"bi", "ky"},"st"}},
```

```
(* ky-bi-chl *)
{(* ky-bi edge *)
{1,   2, 0.9510, 6.00, 584.7, {"bi",  "ky"},"chl"},
{1,   2, 0.9540, 6.00, 584.9, {"bi",  "ky"},"chl"},
{1,   2, 0.9560, 6.00, 585.0, {"bi",  "ky"},"chl"},
{1,   2, 0.9570, 6.00, 585.1, {"bi",  "ky"},"chl"},
{1,   2, 0.9590, 6.00, 585.2, {"bi",  "ky"},"chl"},
{1,   2, 0.9600, 6.00, 585.3, {"bi",  "ky"},"chl"},
{1,   2, 0.9620, 6.00, 585.4, {"bi",  "ky"},"chl"},
{1,   2, 0.9630, 6.00, 585.5, {"bi",  "ky"},"chl"}},

{(* ky-chl edge *)
{1,   2, 0.9520, 6.00, 584.7, {"chl",  "ky"},"bi"},
{1,   2, 0.9550, 6.00, 584.9, {"chl",  "ky"},"bi"},
{1,   2, 0.9560, 6.00, 585.0, {"chl",  "ky"},"bi"},
{1,   2, 0.9580, 6.00, 585.1, {"chl",  "ky"},"bi"},
{1,   2, 0.9590, 6.00, 585.2, {"chl",  "ky"},"bi"},
{1,   2, 0.9600, 6.00, 585.3, {"chl",  "ky"},"bi"},
{1,   2, 0.9620, 6.00, 585.4, {"chl",  "ky"},"bi"},
{1,   2, 0.9630, 6.00, 585.5, {"chl",  "ky"},"bi"}},

(* sill-st-bi *)
{(* st-bi edge *)
{1,   2, 0.2200, 6.00, 645.4, {"st",  "bi"},"sill"},
{1,   2, 0.2400, 6.00, 644.6, {"st",  "bi"},"sill"},
{1,   2, 0.2600, 6.00, 643.8, {"st",  "bi"},"sill"},
{1,   2, 0.2800, 6.00, 643.0, {"st",  "bi"},"sill"},
{1,   2, 0.3000, 6.00, 642.0, {"st",  "bi"},"sill"},
{1,   2, 0.3200, 6.00, 641.0, {"st",  "bi"},"sill"},
{1,   2, 0.3400, 6.00, 639.9, {"st",  "bi"},"sill"},
{1,   2, 0.3600, 6.00, 638.7, {"st",  "bi"},"sill"},
{1,   2, 0.3800, 6.00, 637.4, {"st",  "bi"},"sill"},
{1,   2, 0.4000, 6.00, 636.0, {"st",  "bi"},"sill"},
{1,   2, 0.4200, 6.00, 634.4, {"st",  "bi"},"sill"},
{1,   2, 0.4400, 6.00, 632.7, {"st",  "bi"},"sill"},
{1,   2, 0.4600, 6.00, 630.7, {"st",  "bi"},"sill"},
{1,   2, 0.4800, 6.00, 628.6, {"st",  "bi"},"sill"},
{1,   2, 0.5000, 6.00, 626.1, {"st",  "bi"},"sill"},
{1,   2, 0.5200, 6.00, 623.4, {"st",  "bi"},"sill"}},

{(* sill-bi edge *)
{1,   2, 0.5800, 6.00, 645.3, {"bi",  "sill"},"st"},
{1,   2, 0.6000, 6.00, 645.1, {"bi",  "sill"},"st"},
{1,   2, 0.6200, 6.00, 644.9, {"bi",  "sill"},"st"},
{1,   2, 0.6400, 6.00, 644.6, {"bi",  "sill"},"st"},
{1,   2, 0.6600, 6.00, 644.3, {"bi",  "sill"},"st"},
{1,   2, 0.6800, 6.00, 644.0, {"bi",  "sill"},"st"},
{1,   2, 0.7000, 6.00, 643.7, {"bi",  "sill"},"st"},
{1,   2, 0.7200, 6.00, 643.2, {"bi",  "sill"},"st"},
{1,   2, 0.7400, 6.00, 642.8, {"bi",  "sill"},"st"},
{1,   2, 0.7600, 6.00, 642.2, {"bi",  "sill"},"st"},
{1,   2, 0.7800, 6.00, 641.5, {"bi",  "sill"},"st"},
{1,   2, 0.8000, 6.00, 640.7, {"bi",  "sill"},"st"},
{1,   2, 0.8200, 6.00, 639.7, {"bi",  "sill"},"st"},
{1,   2, 0.8400, 6.00, 638.5, {"bi",  "sill"},"st"},
{1,   2, 0.8600, 6.00, 636.9, {"bi",  "sill"},"st"},
{1,   2, 0.8800, 6.00, 634.6, {"bi",  "sill"},"st"},
{1,   2, 0.9000, 6.00, 631.5, {"bi",  "sill"},"st"},
{1,   2, 0.9200, 6.00, 626.7, {"bi",  "sill"},"st"},
{1,   2, 0.9400, 6.00, 618.5, {"bi",  "sill"},"st"}},
```

```
(* st-g-bi *)
{(* g-bi edge *)
{1,   2, 0.1590, 6.00, 628.2, {"g", "bi"},"st"},
{1,   2, 0.1600, 6.00, 629.3, {"g", "bi"},"st"},
{1,   2, 0.1700, 6.00, 636.9, {"g", "bi"},"st"},
{1,   2, 0.1800, 6.00, 644.9, {"g", "bi"},"st"},
{1,   2, 0.1900, 6.00, 653.2, {"g", "bi"},"st"}},

{(* st-bi edge *)
{1,   2, 0.1590, 6.00, 628.2, {"st", "bi"},"g"},
{1,   2, 0.1600, 6.00, 628.7, {"st", "bi"},"g"},
{1,   2, 0.1700, 6.00, 630.9, {"st", "bi"},"g"},
{1,   2, 0.1800, 6.00, 633.1, {"st", "bi"},"g"},
{1,   2, 0.1900, 6.00, 635.4, {"st", "bi"},"g"},
{1,   2, 0.2000, 6.00, 637.8, {"st", "bi"},"g"},
{1,   2, 0.2100, 6.00, 640.2, {"st", "bi"},"g"},
{1,   2, 0.2200, 6.00, 642.7, {"st", "bi"},"g"},
{1,   2, 0.2300, 6.00, 645.4, {"st", "bi"},"g"}},

(* sill-g-bi *)
{(* g-bi edge *)
{1,   2, 0.1740, 6.00, 651.3, {"g", "bi"},"sill"},
{1,   2, 0.1760, 6.00, 649.0, {"g", "bi"},"sill"},
{1,   2, 0.1780, 6.00, 646.6, {"g", "bi"},"sill"},
{1,   2, 0.1800, 6.00, 644.3, {"g", "bi"},"sill"}},

{(* sill-bi edge *)
{1,   2, 0.5200, 6.00, 650.5, {"bi", "sill"},"g"},
{1,   2, 0.5300, 6.00, 649.9, {"bi", "sill"},"g"},
{1,   2, 0.5400, 6.00, 649.3, {"bi", "sill"},"g"},
{1,   2, 0.5500, 6.00, 648.7, {"bi", "sill"},"g"},
{1,   2, 0.5600, 6.00, 648.1, {"bi", "sill"},"g"},
{1,   2, 0.5700, 6.00, 647.4, {"bi", "sill"},"g"},
{1,   2, 0.5800, 6.00, 646.7, {"bi", "sill"},"g"},
{1,   2, 0.5900, 6.00, 645.9, {"bi", "sill"},"g"},
{1,   2, 0.6000, 6.00, 645.1, {"bi", "sill"},"g"},
{1,   2, 0.6100, 6.00, 644.1, {"bi", "sill"},"g"}} };

allqlines = {
(* chl *)
{(* bi-chl edge *)
{1,   2, 0.3400, 6.00, 499.3, {"chl"},"bi"},
{1,   2, 0.3500, 6.00, 506.7, {"chl"},"bi"},
{1,   2, 0.3600, 6.00, 514.5, {"chl"},"bi"},
{1,   2, 0.3700, 6.00, 522.5, {"chl"},"bi"},
{1,   2, 0.3800, 6.00, 531.1, {"chl"},"bi"},
{1,   2, 0.3900, 6.00, 540.1, {"chl"},"bi"},
{1,   2, 0.4000, 6.00, 549.6, {"chl"},"bi"},
{1,   2, 0.4100, 6.00, 559.6, {"chl"},"bi"},
{1,   2, 0.4200, 6.00, 570.4, {"chl"},"bi"},
{1,   2, 0.4300, 6.00, 581.8, {"chl"},"bi"},
{1,   2, 0.4400, 6.00, 594.1, {"chl"},"bi"}},

{(* st-chl edge *)
{1,   2, 0.4000, 6.00, 620.7, {"chl"},"st"},
{1,   2, 0.4100, 6.00, 600.0, {"chl"},"st"},
{1,   2, 0.4200, 6.00, 579.4, {"chl"},"st"},
{1,   2, 0.4300, 6.00, 558.6, {"chl"},"st"},
{1,   2, 0.4400, 6.00, 537.5, {"chl"},"st"},
{1,   2, 0.4500, 6.00, 516.0, {"chl"},"st"}},
```

```
{(* ctd-chl edge *)
{1,   2, 0.4350, 6.00, 563.1, {"chl"},"ctd"},
{1,   2, 0.4360, 6.00, 551.1, {"chl"},"ctd"},
{1,   2, 0.4370, 6.00, 539.3, {"chl"},"ctd"},
{1,   2, 0.4380, 6.00, 527.5, {"chl"},"ctd"},
{1,   2, 0.4390, 6.00, 515.8, {"chl"},"ctd"},
{1,   2, 0.4400, 6.00, 504.2, {"chl"},"ctd"},
{1,   2, 0.4410, 6.00, 492.6, {"chl"},"ctd"}},

(* bi *)
{(* bi-chl edge *)
{1,   2, 0.0700, 6.00, 496.4, {"bi"},"chl"},
{1,   2, 0.0800, 6.00, 507.5, {"bi"},"chl"},
{1,   2, 0.0900, 6.00, 518.2, {"bi"},"chl"},
{1,   2, 0.1000, 6.00, 528.6, {"bi"},"chl"},
{1,   2, 0.1100, 6.00, 538.8, {"bi"},"chl"},
{1,   2, 0.1200, 6.00, 548.9, {"bi"},"chl"},
{1,   2, 0.1300, 6.00, 558.8, {"bi"},"chl"},
{1,   2, 0.1400, 6.00, 568.8, {"bi"},"chl"},
{1,   2, 0.1500, 6.00, 578.7, {"bi"},"chl"},
{1,   2, 0.1600, 6.00, 588.7, {"bi"},"chl"}},

{(* st-bi edge *)
{1,   2, 0.1440, 6.00, 567.8, {"bi"},"st"},
{1,   2, 0.1467, 6.00, 578.1, {"bi"},"st"},
{1,   2, 0.1493, 6.00, 588.6, {"bi"},"st"},
{1,   2, 0.1520, 6.00, 599.4, {"bi"},"st"},
{1,   2, 0.1547, 6.00, 610.1, {"bi"},"st"},
{1,   2, 0.1573, 6.00, 621.4, {"bi"},"st"},
{1,   2, 0.1600, 6.00, 632.5, {"bi"},"st"}},

{(* g-bi edge *)
{1,   2, 0.1580, 6.00, 622.5, {"bi"},"g"},
{1,   2, 0.1590, 6.00, 628.0, {"bi"},"g"},
{1,   2, 0.1600, 6.00, 634.1, {"bi"},"g"},
{1,   2, 0.1610, 6.00, 640.0, {"bi"},"g"},
{1,   2, 0.1620, 6.00, 645.9, {"bi"},"g"},
{1,   2, 0.1630, 6.00, 651.8, {"bi"},"g"},
{1,   2, 0.1640, 6.00, 657.8, {"bi"},"g"}},

{(* bi-ksp edge *)
{1,   2, 0.0300, 6.00, 494.0, {"bi"},"ksp"},
{1,   2, 0.0400, 6.00, 514.8, {"bi"},"ksp"},
{1,   2, 0.0500, 6.00, 533.7, {"bi"},"ksp"},
{1,   2, 0.0600, 6.00, 551.5, {"bi"},"ksp"},
{1,   2, 0.0700, 6.00, 568.6, {"bi"},"ksp"},
{1,   2, 0.0800, 6.00, 585.1, {"bi"},"ksp"},
{1,   2, 0.0900, 6.00, 601.6, {"bi"},"ksp"},
{1,   2, 0.1000, 6.00, 617.8, {"bi"},"ksp"},
{1,   2, 0.1100, 6.00, 634.1, {"bi"},"ksp"},
{1,   2, 0.1200, 6.00, 650.5, {"bi"},"ksp"}},

(* als *)
{(* ky-chl edge *)
{1,   2, 0.9600, 6.00, 603.6, {"ky"},"chl"},
{1,   2, 0.9650, 6.00, 578.6, {"ky"},"chl"},
{1,   2, 0.9700, 6.00, 552.6, {"ky"},"chl"},
{1,   2, 0.9750, 6.00, 524.8, {"ky"},"chl"},
{1,   2, 0.9800, 6.00, 494.4, {"ky"},"chl"}},
```

```
{(* ky-bi edge *)
{1,   2, 0.9635, 6.00, 633.8, {"ky"},"bi"},
{1,   2, 0.9635, 6.00, 622.2, {"ky"},"bi"},
{1,   2, 0.9635, 6.00, 614.0, {"ky"},"bi"},
{1,   2, 0.9636, 6.00, 605.7, {"ky"},"bi"},
{1,   2, 0.9636, 6.00, 597.9, {"ky"},"bi"},
{1,   2, 0.9636, 6.00, 591.0, {"ky"},"bi"},
{1,   2, 0.9637, 6.00, 584.5, {"ky"},"bi"},
{1,   2, 0.9637, 6.00, 577.8, {"ky"},"bi"}},

{(* sill-bi edge *)
{1,   2, 0.9622, 6.00, 655.6, {"sill"},"bi"},
{1,   2, 0.9624, 6.00, 650.5, {"sill"},"bi"},
{1,   2, 0.9626, 6.00, 645.4, {"sill"},"bi"},
{1,   2, 0.9628, 6.00, 640.4, {"sill"},"bi"},
{1,   2, 0.9630, 6.00, 635.5, {"sill"},"bi"},
{1,   2, 0.9632, 6.00, 630.6, {"sill"},"bi"},
{1,   2, 0.9634, 6.00, 625.8, {"sill"},"bi"},
{1,   2, 0.9636, 6.00, 621.0, {"sill"},"bi"}},

{{1,  2,      2,    6,    400, {"ky"},"Q"},   (* forces drawing properly  *)
{1,  2,      2,    6,    623.4, {"ky"},"Q"}},

{{1,  2,      2,    6,    623.4, {"sill"},"Q"},
{1,  2,      2,    6,    800, {"sill"},"Q"}}  };
```

☐ assembling data

```
setupvx;
```

■ drawing diagrams

```
left = 0; right = 1; bottom = 500; top = 650;
delv = 2;
makevx[6.00];
```
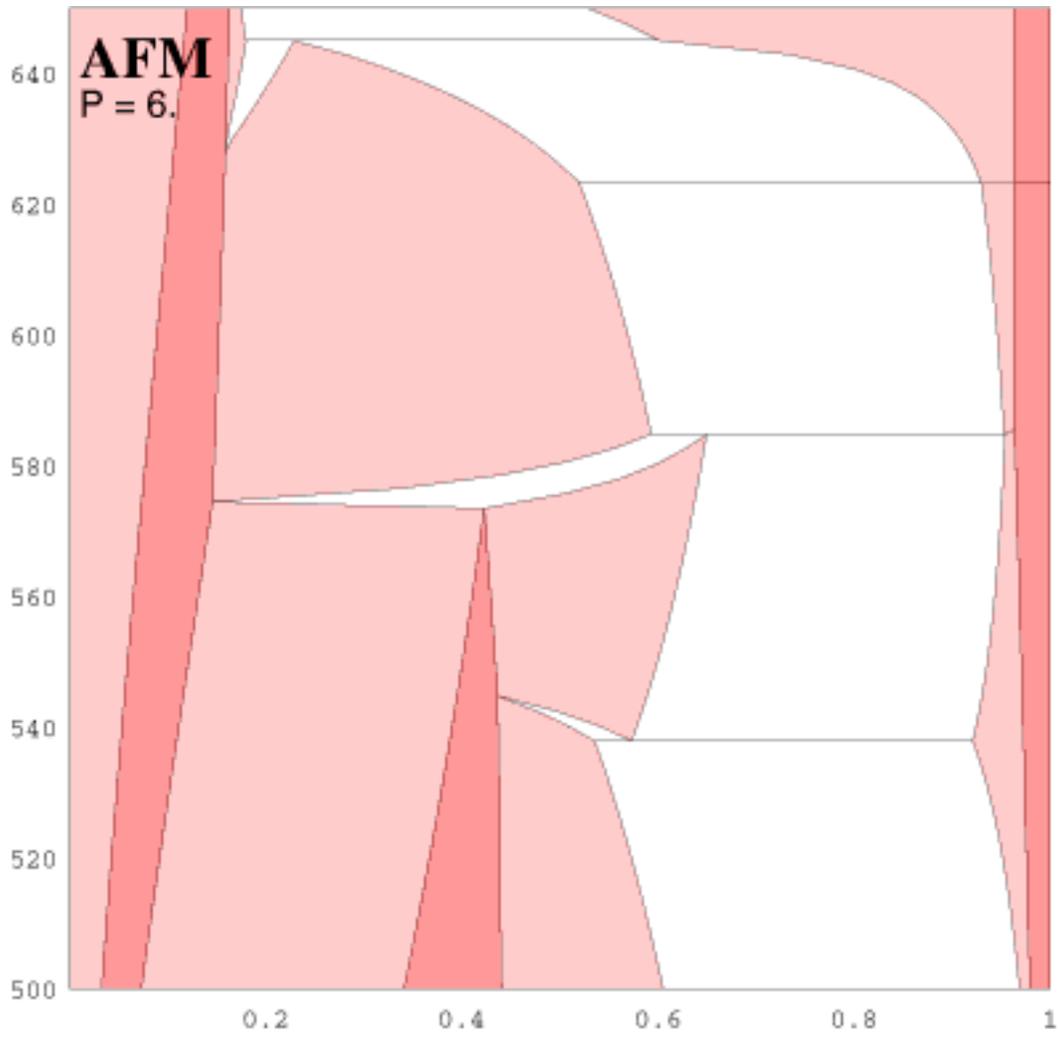

AFM
P = 6.

AFM (+ mu + q + H2O) 6 kbar, $x_{Fe} = 0.6$

T (°C)

g sill
st bi
bi sill
sill
bi af
bi g
sill
ky
bi ky
bi st
ky bi
st chl
bi
ky
st chl
st ky
bi chl
st chl
ctd ky
ctd ky
chl
chl ctd

Al/(Al + Fe + Mg)
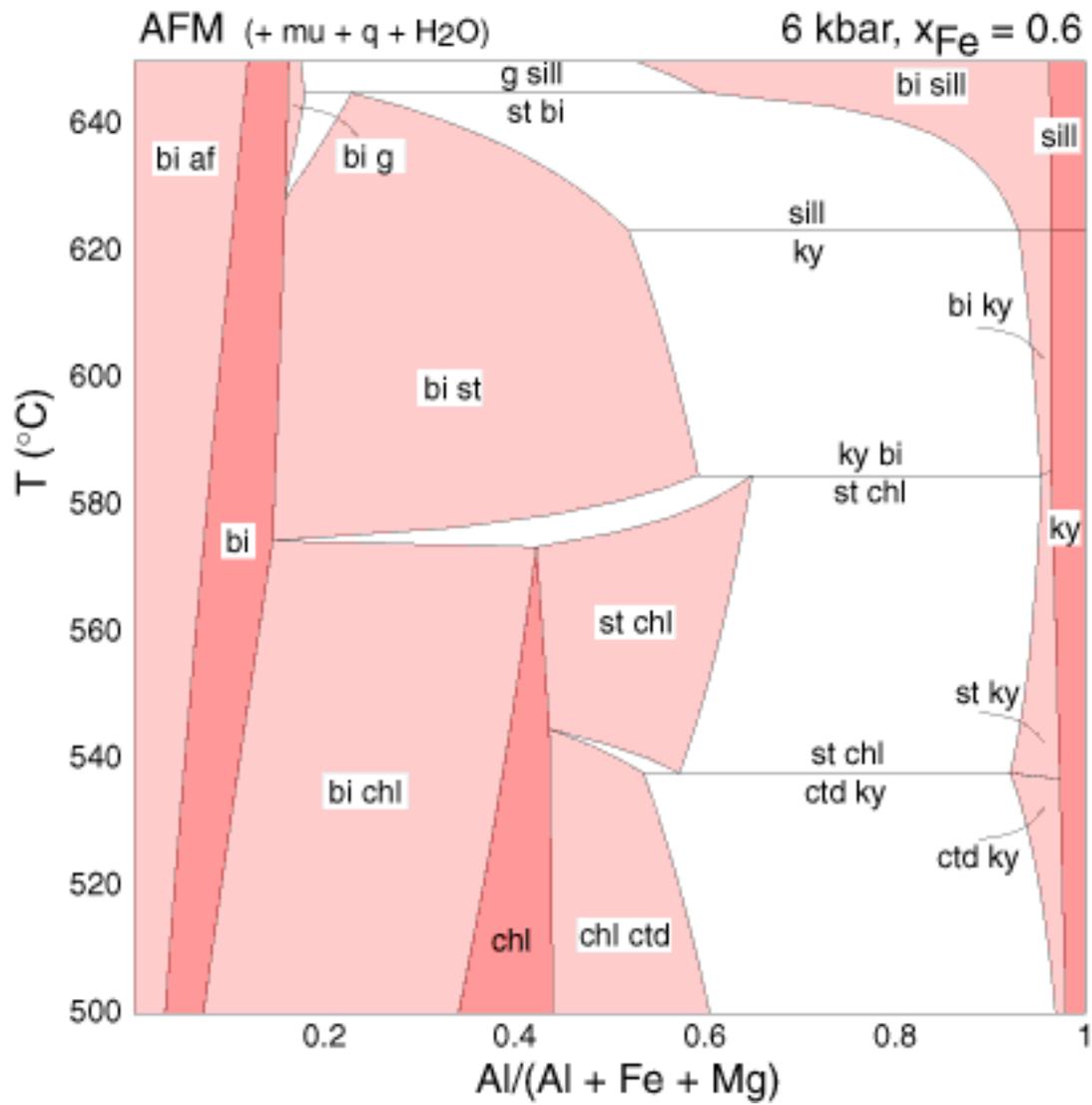
Annotated THERMOCALC logfiles

AFM projection calculations

In this example we wish to calculate the compositions of minerals in a divariant assemblage to plot onto a Thompson AFM projection. The program accepts the names of the phases to project from (mu, q, H2O) and prompts for the names and compositions of the corners of the projection plane (AFM). The projection is always made from the equilibrium compositions of the projection phases, not pure muscovite. A script line in the datafile is used to request projections, and is entered there as:

     project ask

Th following figure shows the constructional features of an AFM compatibility diagram.
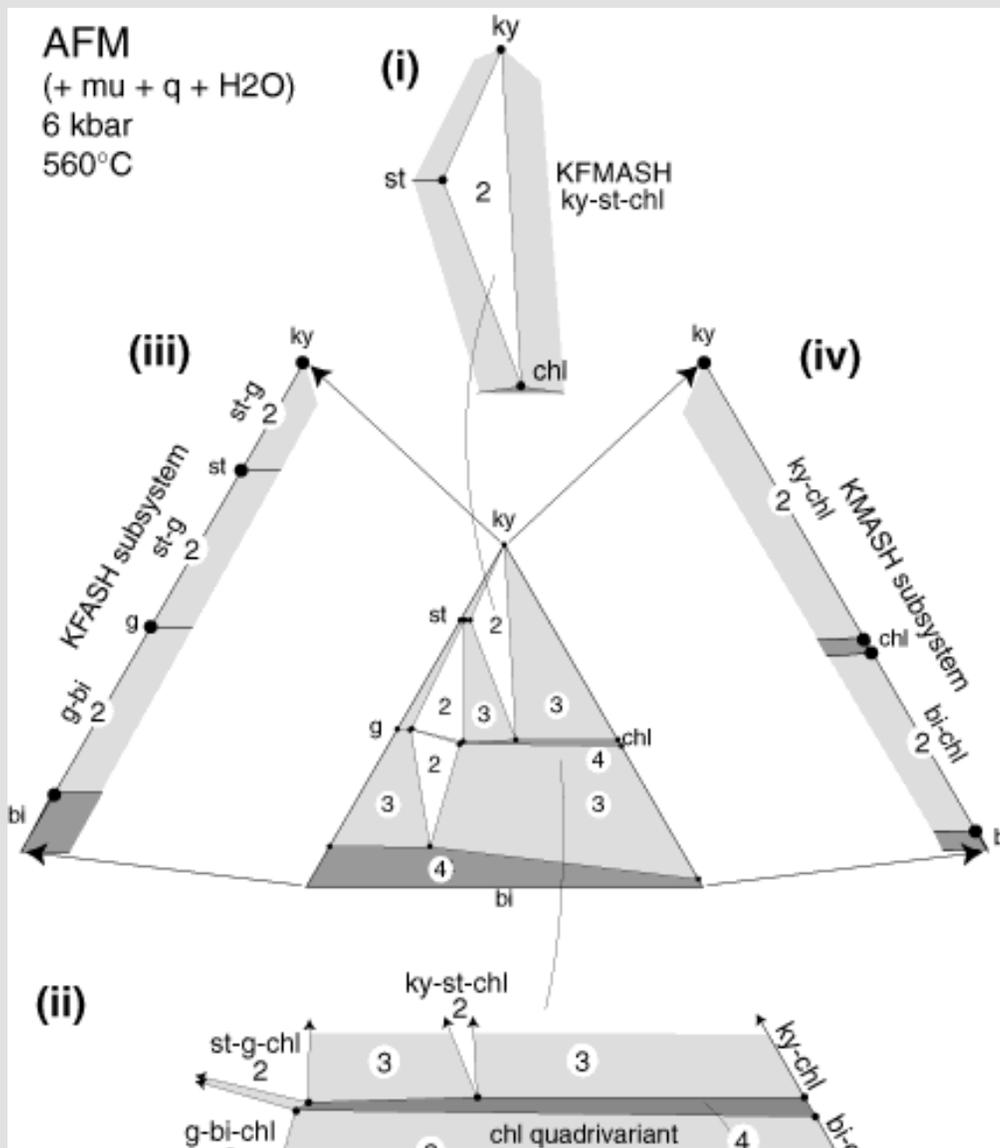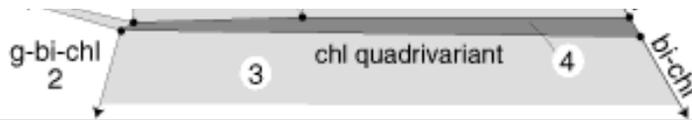
As can be seen in the figure, the main defining feature of the geometry of an AFM diagram, are the corners of the tie triangles or divariants (labelled 2), in the full-system and, for the edges, in the subsystems. So calculation of the divariants is a central part of calculating compatibility diagrams. The edges of the trivariants in systems such as this tend to be straight, so that calculating their exact positions is not necessary. However the approach used is illustrated at the end of this example.

For the following, it is assumed that everything has been done exactly as in the previous divariant example (in PT projection example) until this prompt:

```
...
specification of PT window:
P range over which equilibria to be calculated
P window: P low,high :  6
```

Only one pressure in (kbar) entered. For a range in P, two pressures would need to be entered here, and you would then be prompted for the interval

```
T range over which equilibria to be calculated
T window: T low,high :  560
```

Again, only one temperature in °C. We are only interested in 6 kbar, 560°C. For a range in T, two temperatures would need to be entered here, and you would then be prompted for the interval

```
project mineral compositions onto a compatibility diagram ? yes
```

yes, we want to do projection in this run (from mu+q+H2O, as specified as being in excess in the script in the datafile)

```
projection plane has 3 apices, leaving Al2O3 MgO FeO K2O
to be represented by mu and the projection plane
compositions of the 3 apices are needed in terms of:
  Al2O3 MgO FeO K2O

specify apices:
    0: by oxide list (when each apex is just an oxide)
    1: apex by apex (when some apices are composite)
code :  0
oxide list (3 indices) :   1 3 2
```

entering the apices from the list of oxides given above, in the order given in that list, i.e. 1 3 2 means Al2O3 FeO MgO

the alternative way to do this is to use the apex by apex option, as illustrated below. The output picks up from the same point where the "specify apices" prompt occurred above:

```
        specify apices:
            0: by oxide list (when each apex is just an oxide)
            1: apex by apex (when some apices are composite)
        code : 1
        1st apex name : A
        apex composition :  1 0 0 0
        2nd apex name : F
        apex composition :  0 0 1 0
        3rd apex name : M
        apex composition :  0 1 0 0
```

```
projection plane
         Al2O3        MgO       FeO       K2O
A        1.000          0         0         0
F            0          0     1.000         0
M            0      1.000         0         0
<=====================================================>
phases : g, chl, bi, (mu, q, fluid)
reactions :  |X|X|XXX|XX
```

At each selected P and T, the calculated compositional parameters are listed as usual, but now the phase compositions are also given in terms of the A, F and M coordinates as set out in the table below:

```
-------------------------------------------------------------------

 P(kbar)       T(°C)        x(g)     x(chl)     y(chl)     x(bi)      y(bi)     x(mu)     y(mu)
    6.00       560.0      0.9388     0.6894     0.5712     0.7190     0.3816    0.8638    0.8366

proj          A         F         M        mu     phase
g         0.250     0.704     0.046            -0.250
chl       0.190     0.558     0.251            -0.167
bi       -0.227     0.871     0.357     0.500  -0.500
```

for each phase, the numbers given are the reaction coefficients for the phase in terms of the projecting phase(s) and A, F and M, normalised so the reaction coefficients A, F and M sum to one. These are the AFM coordinates. So, for bi, the reaction is

$$0.5 \text{ bi} + 0.227 \text{ A} = 0.5 \text{ mu} + 0.871 \text{ F} + 0.357 \text{ M}$$

Note that the projected positions of the phases are from *this* calculated composition of muscovite; across a calculated composition diagram, each tie triangle is projected from its own calculated muscovite composition.

If the phase in fact plots at infinity (as does K-feldspar in the AFM projection), the back-projected position is given, but the output line ends with a bullet, flagging the "illegality" of this.

```
more phase diagram calculations ? no
```

no more mode 1 calculations wanted

```
all done ? yes
```

yes, finished with using THERMOCALC

For succeeding runs with this projection plane, the projection plane information can be entered in the datafile via scripts. These scripts are provided in the logfile for any run in which a plane was generated interactively, as in the above. It can then be cut from the logfile and pasted into the datafile. In this case the scripts are

```
% [script to enter the projection plane info]
% -------------------------------------------------
setproject     A   1 0 0 0
setproject     F   0 0 1 0
setproject ask M   0 1 0 0
% -------------------------------------------------
```

You may run the program exactly as in the above, and the output will be exactly as above without you having been prompted for the compositions or names of the apices. Obviously this is a time-saver. With 'ask' in the setproject script, you will be asked, on running THERMOCALC, if you want to use the projection plane in the datafile. This question is not asked, and the projection plane is used, if the 'ask' is replaced by 'yes' (or omitted).

To calculate the boundaries of a trivariant field, the isopleth facility in THERMOCALC is used, in conjunction with projection. This is accessed by putting

```
setiso ask
```

in the datafile scripts. Now we will look at the boundaries of the chl + bi trivariant.

Starting part way through a run, at the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   bi chl
```

Investigating the bi+chl trivariant in AFM

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
```

```
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 3
```

Calculating a trivariant

```
you will have to set at least 1 compositional variable
you may set compositional variables, from:
  x(chl) y(chl) x(bi) y(bi) x(mu) y(mu)
(maximum number to set = 3)
which variables to set : 1
```

Specifying which compositional variable to set in calculating a series of tie lines across the trivariant:
x(chl) or x(bi) are obvious ones

```
how to specify isopleth for x(chl):
 0: list of values
 1: start, finish, interval
code : 1
isopleth: low,high,interval :  0.2 0.8 0.2
equilibia now effectively divariant
```

The calculations are to be performed for x(chl) = 0.2, 0.4, 0.6 and 0.8

```
specification of PT window:
P range over which equilibria to be calculated
P window: P low,high : 6
T range over which equilibria to be calculated
T window: T low,high : 560
```

The calculations are to be performed at 6 kbar and 560°C

```
project mineral compositions onto a compatibility diagram ? yes

use projection plane specified in datafile ? yes
projection plane has 3 apices, leaving Al2O3 MgO FeO K2O
to be represented by mu and the projection plane
projection plane (from script)
          Al2O3       MgO       FeO       K2O
A         1.000         0         0         0
F             0         0     1.000         0
M             0     1.000         0         0
```

The projection plane to be used was entered as shown above as a script in the datafile

```
<=================================================>
phases : chl, bi, (mu, q, fluid)
reactions : |XXX|X|X
```

The coordinates of a series of bi - chl tie lines, corresponding to the x(chl) values chosen, are calculated.

```
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
   6.00       560.0       0.2    0.5553    0.2237    0.3710    0.4167    0.8761

proj       A         F         M        mu     phase
chl     0.185     0.163     0.652              -0.167
bi     -0.253     0.268     0.984     0.500    -0.500
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
   6.00       560.0       0.4    0.5617    0.4345    0.3750    0.6558    0.8575

proj       A         F         M        mu     phase
chl     0.187     0.325     0.488              -0.167
bi     -0.241     0.524     0.718     0.500    -0.500
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
   6.00       560.0       0.6    0.5682    0.6336    0.3795    0.8109    0.8424

proj       A         F         M        mu     phase
chl     0.189     0.486     0.324              -0.167
bi     -0.231     0.766     0.465     0.500    -0.500
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
   6.00       560.0       0.8    0.5749    0.8218    0.3843    0.9196    0.8301

proj       A         F         M        mu     phase
chl     0.192     0.647     0.162              -0.167
bi     -0.223     0.997     0.226     0.500    -0.500

more phase diagram calculations ? no
```

no more mode 1 calculations wanted

```
all done ? yes
```

yes, finished with using THERMOCALC

[back to log list | back to start]

Annotated THERMOCALC logfiles

Isopleth in a divariant field in PT

We wish to calculate the isopleths (lines of constant composition) for almandine content in garnet in the assemblage garnet + kyanite + biotite + muscovite + quartz. These will be lines on a PT projection. Running the program for isopleths requires setting a script in the datafile as follows

setiso yes (or ask)

```
THERMOCALC v2.5, © Roger Powell and Tim Holland running at 21.50 on Thu 5 Dec,1996
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)

calculation type :
     0 = table of thermodynamic data of end-members
     1 = phase diagram calculations
     2 = average pressure-temperature calculations
     3 = calculations on all reactions between end-members
     4 = list end-member names and compositions
control code   : 1
```

means do mode 1 phase diagram calculations

```
data filename : suffix to "th d" : st
```

use the data in the file th dst

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O

log output will be found in "th log" (from prefs)
output will be found in the file, "th ost" (from prefs)
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
output will be found in the file, "th math" (from prefs)

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :  g bi ky mu q H2O
```

means use these phases only; you could, more efficiently, say omit st chl. Or given that the calculation involves mu, q and H2O being in excess (set immediately below), the entered phases could be just g bi ky (and THERMOCALC substitutes the inexcess phases)

```
fluid is in excess (from script)
```

```
use in excess phases specified in datafile ? yes
```

yes, take the names from the script in the datafile (in script)

```
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance : 2
```

divariant equilibrium wanted

```
do you want to set any compositional variables (eg to calculate isopleths) ? yes
```

yes, we do want to set the garnet x(g) variable

```
you may set compositional variables, from:x(g) x(bi) y(bi) x(mu) y(mu)
(maximum number to set = 2)
which variables to set : x(g)
```

We could have entered 1 here, meaning the first in the list.

```
how to specify isopleth for x(g):
 0: list of values
 1: start, finish, interval
code : 1
isopleth: low,high,interval :  0.8 0.95 0.05
```

we want to set x(g) at values of 0.8, 0.85, 0.9 and 0.95.

```
equilibia now effectively univariant (eg is a line in PT)
```

An isopleth in a divariant field is a line (effectively univariant)

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :  5 10
```

calculate T at pressures in the range 5 to 10 kbar

```
T window within which reactions expected to lie
T window: T low,high : (nothing input)
```

by hitting return, the T window for calculated T's is the default T range

```
P window :5 <-> 10 kbar :P interval : 1
```

calculate T every 1 kbar between 5 and 10 kbar

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

In the table below, the program lists the temperature for each pressure and each set x(g) as well as the composition of the other phases in the assemblage.

As seen below, the x(g)=0.85 isopleth runs through 870°C at 5 kbar, 620°C at 7 kbar and 458°C at 10 kbar pressure.

Where the program has not been able to find a (satisfactory) solution it has printed a code number in the leftmost column (e.g. the zero on the first line of the table). A value of 0 indicates that the calculated temperature lies outside the window selected above, 1 (and larger) that no solution could be found to the non-linear equations during calculation.

```
phases : g, bi, ky, (mu, q, fluid)
reactions : |XXX|XX
 P(kbar)      T(°C)      x(g)      x(bi)      y(bi)      x(mu)      y(mu)
0
      5.0        870      0.85      0.635      0.606      0.770      0.895
      5.0        620       0.9      0.638      0.497      0.801      0.890
      5.0        388      0.95      0.640      0.343      0.840      0.890
      6.0        915       0.8      0.563      0.595      0.713      0.887
      6.0        716      0.85      0.573      0.516      0.745      0.881
      6.0        529       0.9      0.579      0.413      0.779      0.876
      6.0        337      0.95      0.579      0.265      0.820      0.874

      7.0        783       0.8      0.513      0.519      0.692      0.872
      7.0        620      0.85      0.520      0.437      0.724      0.865
      7.0        466       0.9      0.526      0.339      0.759      0.860
0
      8.0        685       0.8      0.465      0.444      0.671      0.854
      8.0        553      0.85      0.474      0.368      0.705      0.848
      8.0        419       0.9      0.477      0.272      0.742      0.840
0
      9.0        616       0.8      0.425      0.378      0.654      0.836
      9.0        501      0.85      0.432      0.304      0.688      0.828
      9.0        381       0.9      0.433      0.214      0.726      0.818
0
     10.0        562       0.8      0.388      0.318      0.639      0.816
     10.0        458      0.85      0.393      0.247      0.673      0.805
     10.0        349       0.9      0.392      0.165      0.711      0.791
1
more phase diagram calculations ? no
```

no more mode 1 calculations wanted

all done ? yes

finished with THERMOCALC

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Annotated THERMOCALC logfiles

Setting bulk compositions

This example shows how to specify bulk compositions and how to enter them as scripts in datafiles. This is essential for calculating pseudosections showing the assemblages "seen" by a particular bulk composition.

```
THERMOCALC v2.5, © Roger Powell and Tim Holland running at 17.18 on Fri 6 Dec,1996

(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)

calculation type :
     0 = table of thermodynamic data of end-members
     1 = phase diagram calculations
     2 = average pressure-temperature calculations
     3 = calculations on all reactions between end-members
     4 = list end-member names and compositions
control code  : 1
```

means do mode 1 phase diagram calculations

```
data filename : suffix to "th d" : st
```

filename to use is th dst

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O

log output will be found in "th log" (from prefs)
output will be found in the file, "th ost" (from prefs)
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
output will be found in the file, "th math" (from prefs)

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky
```

this time we want to calculate the ky-absent reaction

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
```

yes, take the names from the script in the datafile (from script)

```
phases in excess: mu q  (from script)
```

```
variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 1
read in bulk compositions and
generate pseudosection information for them ? yes
```

yes, we want to use bulk composition info, for example, for pseudosection calculations (from script).

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :   6 12
T window within which reactions expected to lie
T window: T low,high : (nothing input)
the T window in which calculated T's are expected to lie.
P window :6 <-> 12 kbar :P interval : 1
```

calculate T between 6 and 12 kbar at 1 kbar intervals

```
project mineral compositions onto a compatibility diagram ? no

specifying bulk compositions

how to specify bulk compositions:
 0: one composition - in terms of components (oxides)
 1: on a line between two points - in terms of components (oxides)
 2: on a line between two points - in terms of mineral end-members
 3: one composition - in terms of 'real' phase compositions
code : 3
```

we will determine a suitable bulk composition based on the composition of garnet, chlorite, biotite and muscovite in an assemblage as an example.

```
components to be specified : Al2O3 MgO FeO K2O

relevant phases : st g chl bi mu

which phases to define composition (divariant is 4 phases) :   2 3 4 5
we will provide compositions for all phases except the first (st)
using : g chl bi mu
specifying compositions of (solid) solutions:
for g
  value for x(g) : 0.9
```

```
for chl
  value for x(chl) : 0.55
  value for y(chl) : 0.6
for bi
  value for x(bi) : 0.55
  value for y(bi) : 0.4
for mu
  value for x(mu) : 0.8
  value for y(mu) : 0.9
```

the values for x(i) and y(i) compositional variables for each of the phases has been entered at the prompts. These compositions might, for example, come from your own probe data, or from the results of a previous THERMOCALC calculation.

```
proportions (the resulting composition will be normalised to 100) : 10 30 25 35
```

the modal proportions (molar, on a 1 oxide basis) are entered here, i.e. 10% garnet, 30% chlorite, 25% biotite and 35% muscovite.

The program converts the info given into a bulk composition in terms of oxide proportions.

```
composition
 Al2O3   MgO    FeO    K2O
 38.62  19.21  30.29  11.88
```

... and then THERMOCALC performs the calculations with this bulk composition

The script info, to allow calculations with this bulk composition to be performed without having to enter the information again, can be "cut" from the log file and "pasted" into the input file 'th dst'. The script looks like this:

```
% [script to enter the bulk composition info]
% ------------------------------------------------
%               Al2O3    MgO     FeO     K2O
setbulk ask    38.62   19.21   30.29   11.88
% ------------------------------------------------
```

If a bulk composition is already available, for example from XRF data, then it can be entered directly into THERMOCALC using the zero option at the "how to specify bulk compositions" prompt. Or, more easily, it can be entered directly into the datafile by copying the form of the script just given.

It is worth noting that using XRF analyses directly can be disappointing if the "equilibration volume" in which the equilibrium mineral assemblage observed in a rock does not include, for

example, the interior parts of porphyroblasts. In such circumstances it can be more helpful to use the approach used above, and generate the bulk composition from the compositions of the observed minerals, thus forcing the resulting bulk composition to lie within the "compositional polygon" defined by the minerals. In an extension of this idea, the results of a THERMOCALC calculation can be used as input to the above, to generate a bulk composition. In this way one can generate a bulk composition that does, for example, see a particular equilibrium (say, cross a particular univariant at a particular PT). Although the logic is potentially circular if the calculations are being used to investigate the PT path of rocks, it nevertheless provides a starting point for such calculations.

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Annotated THERMOCALC logfiles

PT pseudosection

We now show how to generate a PT pseudosection, for a single bulk composition entered into the datafile with the script:

```
% [script to enter the bulk composition info]
% -------------------------------------------------
%                 Al2O3    MgO    FeO    K2O
setbulk yes    41.89  18.19  27.29  12.63
% -------------------------------------------------
```

This is the bulk composition used for the PT pseudosection discussed in the body of the paper. The diagram will be built up line by line and point by point, first locating the univariant curve for the staurolite isograd reaction in AFM. Only part of this reaction will be "seen" by our bulk composition because the compositions of the phases in equilibrium at the reaction change along the reaction line. Various constructional features of the PT pseudosection we wish to calculate are shown in the following figure
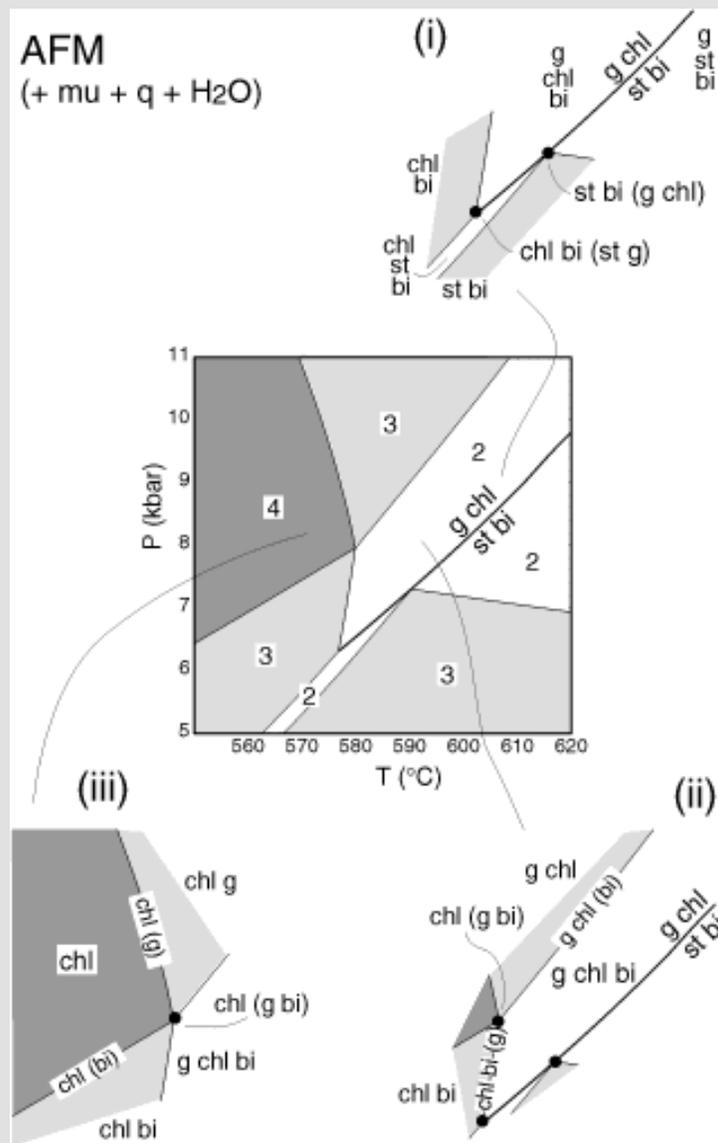
The labelling of points and lines in this figure are in terms of the phases involved in the lower variance assemblage, with the phase(s) in brackets being those that have gone to zero (in going from the lower to the higher variance assemblage) at the point or line. So, in (i) in the figure, the point which is the low P end of the univariant, is denoted bi chl (st g) because the univariant assemblage is g + chl + bi + st, and, at the point, going into the trivariant, the modes of st and g are zero.

Note that on such diagrams the variance changes across lines (but not univariant lines) can only be by one, and that the maximum variance change across a point can only be by two.

```
THERMOCALC v2.5, © Roger Powell and Tim Holland running at 17.18 on Fri 6 Dec,1996

(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)

calculation type :
     0 = table of thermodynamic data of end-members
     1 = phase diagram calculations
     2 = average pressure-temperature calculations
```

```
      3 = calculations on all reactions between end-members
      4 = list end-member names and compositions
control code  : 1
```

means do mode 1 phase diagram calculations

```
data filename : suffix to "th d" : st
```

filename to use is th dst

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O

log output will be found in "th log" (from prefs)
output will be found in the file, "th ost" (from prefs)
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
output will be found in the file, "th math" (from prefs)

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :  omit ky
```

this time we want to calculate the ky-absent reaction

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
```

question answered via the script, setexcess, in the datafile, with the in excess phases given there.

```
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 1
read in bulk compositions and
generate pseudosection information for them ? yes
```

question answered via the script in the datafile, "pseudosection".

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :  6 12
T window within which reactions expected to lie
T window: T low,high : (nothing input)
```

```
the T window in which calculated T's are expected to lie.
P window :6 <-> 12 kbar :P interval : 0.25
```

calculations from 6 to 12 kbars, with a 0.25 kbar interval, using the default T range

```
composition
 Al2O3   MgO    FeO    K2O
 41.89 18.19 27.29 12.63
```

composition provided in a script in the datafile, using "setbulk"

```
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions :  |XX|X|X|XXX|XX
 P(kbar)      T(°C)     x(st)      x(g)    x(chl)   y(chl)     x(bi)     y(bi)     x(mu)
y(mu)

    6.00      572.3    0.9366    0.9109    0.6039    0.5929    0.6378    0.4169    0.8118
0.8602
        19g + 33chl + 72mu = 10st + 72bi + 115q + 112H2O
    6.25      575.9    0.9307    0.9033    0.5844    0.5911    0.6181    0.4130    0.7993
0.8579
        19g + 33chl + 72mu = 10st + 72bi + 115q + 113H2O
```

for 6.00 and 6.25 kbar (above) the reaction does not "see" the bulk composition, and so THERMOCALC simply prints out the P,T, the phase compositions and the balanced reaction as it would normally do

```
--------------------------------------------------------------------
 P(kbar)      T(°C)     x(st)      x(g)    x(chl)   y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    6.50      579.5    0.9246    0.8955    0.5657    0.5893    0.5991    0.4091    0.7868
0.8555
        18g + 33chl + 72mu = 10st + 72bi + 115q + 113H2O

   mode        st         g       chl        bi        mu
                      0.0248    0.4176    0.1049    0.4527
            0.0435              0.3506    0.2014    0.4045
```

Now, at 6.50 kbar (above) the reaction is "seen" by the bulk composition and THERMOCALC prints out the modal information for the reactants and the products at the reaction, as well as the usual univariant reaction info. In this case, when crossing the reaction, staurolite has replaced garnet for assemblages with this bulk composition. The numbers are the modes (ie molar proportions of phases).

Following the reaction up pressure below, it can be seen that the modes of st and g have increased from zero, indicating that the field below the seen end of the reaction is the bi + chl (trivariant) field. With reference to the above figure, the point which is the low P end of the univariant can be labelled chl bi (st g)

```
--------------------------------------------------------------------
 P(kbar)      T(°C)     x(st)      x(g)    x(chl)   y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    6.75      582.9    0.9183    0.8876    0.5476    0.5875    0.5806    0.4052    0.7744
```

```
0.8531
        18g + 34chl + 72mu = 10st + 72bi + 114q + 114H2O

   mode       st        g       chl       bi        mu
                     0.0549   0.3856   0.1084   0.4510
         0.0979             0.2340   0.3258   0.3423
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(st)       x(g)    x(chl)   y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     7.00       586.3    0.9118    0.8796    0.5302    0.5857    0.5627    0.4013    0.7621
0.8507
        18g + 34chl + 72mu = 10st + 72bi + 114q + 115H2O

   mode       st        g       chl       bi        mu
                     0.0825   0.3565   0.1115   0.4495
         0.1491             0.1243   0.4428   0.2838
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(st)       x(g)    x(chl)   y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     7.25       589.7    0.9051    0.8713    0.5134    0.5839    0.5453    0.3974    0.7498
0.8483
        18g + 34chl + 72mu = 10st + 72bi + 114q + 116H2O

   mode       st        g       chl       bi        mu
                     0.1080   0.3297   0.1141   0.4482
         0.1977             0.0201   0.5540   0.2282
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(st)       x(g)    x(chl)   y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     7.50       592.9    0.8982    0.8629    0.4972    0.5821    0.5284    0.3935    0.7376
0.8459
        18g + 34chl + 72mu = 10st + 72bi + 114q + 116H2O

   mode       st        g       chl       bi        mu
                     0.1317   0.3049   0.1164   0.4470
         0.1937   0.0273             0.5478   0.2313
```

Now, at 7.5 kbar (above) the product assemblage has changed. The divariant assemblage on the high temperature side of the univariant reaction is now st+bi+g instead of st+bi+chl. On the low temperature side the assemblage is unchanged (g+bi+chl). At some pressure between 6.75 and 7.0, the molar proportions of both garnet and chlorite will be zero, and this pressure marks the point where the trivariant field st+bi impinges at a (trivariant) point on the univariant reaction. This point can be denoted st bi (g chl), as in the above figure.

```
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(st)       x(g)    x(chl)   y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     7.75       596.1    0.8910    0.8543    0.4815    0.5804    0.5119    0.3896    0.7255
0.8435
        17g + 34chl + 72mu = 10st + 72bi + 114q + 117H2O

   mode       st        g       chl       bi        mu
                     0.1539   0.2817   0.1184   0.4460
```

```
        0.1780  0.0591          0.5154  0.2475
--------------------------------------------------------------
 P(kbar)    T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
    8.00    599.3    0.8837   0.8456   0.4664   0.5786   0.4959   0.3857   0.7134
0.8410
       17g + 34chl + 73mu = 10st + 73bi + 114q + 118H2O

  mode      st        g       chl      bi       mu
              0.1749  0.2598  0.1202  0.4451
       0.1634  0.0889          0.4850  0.2627
--------------------------------------------------------------
 P(kbar)    T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
    8.25    602.4    0.8762   0.8367   0.4517   0.5769   0.4804   0.3818   0.7014
0.8386
       17g + 35chl + 73mu = 10st + 73bi + 114q + 118H2O

  mode      st        g       chl      bi       mu
              0.1947  0.2392  0.1218  0.4443
       0.1497  0.1169          0.4563  0.2770
--------------------------------------------------------------
```

   (with the info from 8.5 to 11 kbar omitted)

```
--------------------------------------------------------------
 P(kbar)    T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
   11.25    635.5    0.7689   0.7180   0.3065   0.5566   0.3235   0.3363   0.5611
0.8088
       15g + 36chl + 74mu = 10st + 74bi + 113q + 125H2O

  mode      st        g       chl      bi       mu
              0.3931  0.0333  0.1367  0.4368
       0.0199  0.3841          0.1817  0.4143
--------------------------------------------------------------
 P(kbar)    T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
   11.50    638.0    0.7586   0.7071   0.2965   0.5550   0.3125   0.3326   0.5497
0.8062
       15g + 36chl + 74mu = 10st + 74bi + 113q + 126H2O

  mode      st        g       chl      bi       mu
              0.4087  0.0169  0.1382  0.4361
       0.0101  0.4042          0.1611  0.4247
--------------------------------------------------------------
 P(kbar)    T(°C)     x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
   11.75    640.4    0.7480   0.6961   0.2867   0.5533   0.3018   0.3290   0.5383
0.8037
       14g + 37chl + 74mu = 10st + 74bi + 113q + 126H2O
```

```
  mode        st        g       chl       bi       mu
                      0.4245   0.0003   0.1399   0.4353
             0.0002   0.4244            0.1403   0.4350
```

P(kbar)	T(°C)	x(st)	x(g)	x(chl)	y(chl)	x(bi)	y(bi)	x(mu)
y(mu)								
12.00	642.8	0.7372	0.6849	0.2772	0.5517	0.2914	0.3253	0.5269
0.8011								

```
         14g + 37chl + 74mu = 10st + 74bi + 113q + 127H2O
```

Now, at 12.0 kbar (above) the reaction no longer "sees" the bulk composition and THERMOCALC stops printing out the modal information. As can be seen above, the proportions of both staurolite and chlorite have been decreasing to zero as pressure rises. Thus the univariant line ends in the trivariant g+bi field between 11.75 and 12 kbar.

```
more phase diagram calculations ? yes
```

We can tell from this output that the univariant stops being seen down pressure at a point where the modes of st and g go to zero, ie bi chl (st g). We calculate this point next.

Now, to locate the point where the univariant terminates at low pressures in the bi + chl trivariant field, bi chl (st g):

```
data filename : suffix to "th d" : st
```

with the usual datafile th dst

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  q  H2O
======================================================

phases ignored this run: ctd cd and sill  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :  omit ky
```

we want to calculate the univariant without ky, ie [ky]

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
```

```
      n = n-variant
variance : 1

read in bulk compositions and
generate pseudosection information for them ? yes

you may set zero modal proportions, from:st g chl bi mu q H2O
which to set :   st g
```

the scripts

```
        setmodeiso yes
        zeromodeiso yes
```

are set in the datafile, and so we are prompted for phases whose mode is to be set to zero. In this case we want to find the point where the univariant terminates at the g+bi trivariant field (where chl+st disappear).

```
equilibia now effectively invariant (eg is a point in PT)

specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : (nothing input)
```

Typing return here is fine because the default P and T windows have been set in the datafile by scripts:

```
        setdefPwindow 1    14
        setdefTwindow 300 900
```

```
use bulk compositions specified in datafile for pseudosection ? yes

 Al2O3   MgO   FeO   K2O
 41.89 18.19 27.29 12.63
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions : |XX|X|X|XXX|XX
------------------------------------------------------------------
 P(kbar)     T(°C)    x(st)     x(g)    x(chl)   y(chl)    x(bi)     y(bi)     x(mu)
y(mu)
    6.31     576.8   0.9292   0.9014   0.5797   0.5906   0.6134   0.4120   0.7962
0.8573

   mode       st        g       chl       bi       mu
              0        0   0.4439   0.1019   0.4543
```

The program has listed the PT location of the univariant where the modes of st and chl have gone to zero, corresponding to point bi chl (g st) in the figure.

The existence of this point, and the presence of the g+bi+chl divariant field to lower T and higher P from the univariant line, tells us that there must be a divariant-trivariant boundary along which the mode of g goes to zero (so it is bi chl (g)), emanating from the PT point just calculated. This

is calculated next.

Now we want to find the divariant-trivariant boundary where the bi+chl field abuts the g+bi+chl field (running down pressure from bi chl (st g)), in other words the bi chl (g) line. To find this curve we calculate the divariant assemblage g+bi+chl and stipulate that the mode of g goes to zero:

      starting with the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky st
```

      do divariant assemblage without these phases

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 2

read in bulk compositions and
generate pseudosection information for them ? yes

you may set zero modal proportions, from:g chl bi mu q H2O
which to set : g
```

      to set the mode for g to zero; this maps out a line in PT space

```
equilibia now effectively univariant (eg is a line in PT)

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :   6.2 8
T window within which reactions expected to lie
T window: T low,high : (nothing input)
P window :4 <-> 6 kbar :P interval : 0.2

use bulk compositions specified in datafile for pseudosection ? yes
composition (from script)
```

```
 Al2O3   MgO    FeO    K2O
 41.89 18.19 27.29 12.63
<=================================================>
phases : st, chl, bi, (mu, q, fluid)
reactions : |X|X|XXX|XX


------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.20      576.6    0.9015   0.5799   0.5937   0.6139   0.4176   0.7960   0.8607

   mode        g       chl       bi       mu
               0     0.4406   0.1084   0.4510
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.40      577.0    0.9013   0.5796   0.5882   0.6130   0.4077   0.7963   0.8545

   mode        g       chl       bi       mu
               0     0.4465  0.09661   0.4569
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.60      577.4    0.9011   0.5793   0.5826   0.6120   0.3979   0.7965   0.8482

   mode        g       chl       bi       mu
               0     0.4525  0.08467   0.4629
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.80      577.9    0.9008   0.5790   0.5771   0.6109   0.3882   0.7966   0.8418

   mode        g       chl       bi       mu
               0     0.4585  0.07259   0.4689
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    7.00      578.2    0.9006   0.5785   0.5716   0.6098   0.3787   0.7968   0.8352

   mode        g       chl       bi       mu
               0     0.4646  0.06037   0.4750
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    7.20      578.6    0.9003   0.5781   0.5661   0.6087   0.3693   0.7969   0.8285

   mode        g       chl       bi       mu
               0     0.4708  0.04799   0.4812
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    7.40      579.0    0.9000   0.5775   0.5606   0.6074   0.3601   0.7969   0.8216

   mode        g       chl       bi       mu
               0     0.4771  0.03546   0.4875
------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    7.60      579.3    0.8996   0.5769   0.5552   0.6061   0.3509   0.7969   0.8146

   mode        g       chl       bi       mu
```

```
           0    0.4834   0.02275    0.4938
---------------------------------------------------------------
 P(kbar)     T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
   7.80      579.7     0.8993    0.5763    0.5497    0.6048    0.3419    0.7969    0.8075

  mode         g        chl        bi        mu
             0    0.4899  0.009867    0.5003
7
```

This output gives the position of the bi chl (g) line. The 7 at the end of this output, to higher pressure, tells us that at 8 kbar, this equilibrium could not be calculated. Looking at the modes we can see why: the mode of bi has gone to zero.

That the mode of bi has gone to zero tells us that the bi chl (g) line has terminated in the chl (g bi) point - where the bi+chl+g divariant meets the chl quadrivariant. We calculate this point next.

We now locate the corner of the chl quadrivariant field where it abuts the divariant and trivariant fields, in other words, chl (bi g). This is accomplished by looking for the divariant assemblage g+bi+chl and setting the modes of both g and bi to be zero

starting with the "which phases" prompt

```
st  g   chl  bi   mu  ky   q   H2O
which phases :   omit ky st

fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance : 2

read in bulk compositions and
generate pseudosection information for them ? yes

you may set zero modal proportions, from:g chl bi mu q H2O
which to set :   g bi
```

here we set modes of g and bi to be zero

```
equilibia now effectively invariant (eg is a point in PT)
```

```
specification of PT window:
PT window within which invariant points expected to lie
T low,high, P low,high : (nothing input)
```

so the default PT range is used

```
use bulk compositions specified in datafile for pseudosection ? yes
composition (from script)
 Al2O3   MgO   FeO   K2O
 41.89 18.19 27.29 12.63
<=================================================>
phases : g, chl, bi, (mu, q, fluid)
reactions : |X|X|XXX|XX
-------------------------------------------------------------
 P(kbar)     T(°C)     x(g)   x(chl)  y(chl)   x(bi)   y(bi)   x(mu)   y(mu)
    7.95     579.9   0.8990  0.5757  0.5457  0.6037  0.3352  0.7969  0.8021

   mode        g       chl       bi       mu
              0    0.4948        0    0.5052
```

the point of interest is located at 8 kbar and 580°C

Now that we know where this point is, we can calculate the trivariant-quadrivariant lines that terminate at this point.

We now locate the boundary of the chl quadrivariant field where it abuts the bi+chl trivariant field, ie the chl (bi) line, by calculating the bi+chl trivariant and setting the mode of bi to zero.

starting with the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky st g
```

we need the trivariant assemblage not involving these phases. Now that the number of phases involved in each assemblage of interest is getting small, we could more easily say here,

```
        which phases :   bi chl
```

and thermocalc will insert the in excess phases into this assemblage

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
```

```
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 3
```

trivariant needed (bi+chl field)

```
read in bulk compositions and
generate pseudosection information for them ? yes

you may set zero modal proportions, from:chl bi mu q H2O
which to set : bi
```

set mode for bi to zero at the field boundary

```
equilibia now effectively univariant (eg is a line in PT)

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :  4 9
T window within which reactions expected to lie
T window: T low,high : (nothing input)
P window :4 <-> 9 kbar :P interval : 1

use bulk compositions specified in datafile for pseudosection ? yes
 Al2O3   MgO   FeO   K2O
 41.89 18.19 27.29 12.63
<==================================================>
phases : chl, bi, (mu, q, fluid)
reactions : |XXX|X|X
```

```
----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    4.00      500.7    0.5786    0.5095    0.6183    0.3098    0.8003    0.8257

  mode        chl        bi         mu
          0.4948         0     0.5052
----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    5.00      521.3    0.5778    0.5194    0.6144    0.3167    0.7993    0.8192

  mode        chl        bi         mu
          0.4948         0     0.5052
----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    6.00      541.4    0.5771    0.5287    0.6106    0.3232    0.7984    0.8131

  mode        chl        bi         mu
          0.4948         0     0.5052
----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
```

```
     7.00        561.2    0.5764    0.5376    0.6070    0.3295    0.7976    0.8073

   mode        chl         bi         mu
        0.4948          0    0.5052
-----------------------------------------------------------------
  P(kbar)       T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
     8.00        580.9    0.5757    0.5461    0.6036    0.3355    0.7968    0.8018

   mode        chl         bi         mu
        0.4948          0    0.5052
-----------------------------------------------------------------
  P(kbar)       T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
     9.00        600.4    0.5751    0.5541    0.6003    0.3413    0.7961    0.7965

   mode        chl         bi         mu
        0.4948          0    0.5052
```

This maps out the edge of the chl quadrivariant field against the bi+chl trivariant. Note that the modes of the phases do not change along the line. This is understandable as muscovite is the only K-bearing phase in the assemblage, so its mode is fixed by the K in the bulk composition.

```
more phase diagram calculations ? no
all done ? yes
```

In this way, moving along lines, calculating points, and so on, the whole of the PT pseudosection can be built up... Sometimes however it is difficult to get started in generating pseudosections, particularly in big systems. Gibbs energy minimisation facilities in THERMOCALC allow a start to be made.

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Annotated THERMOCALC logfiles

Gibbs energy minimisation calculations

Sometimes in pseudosection calculations it is necessary to generate a starting point for the sort of calculations followed in pseudosection calculations, or to just check what has been done. The Gibbs energy minimisation calculations shown here, although rather brutish, allow this to be done. The required script to access this facility is

```
dogmin yes
```

As well, as seen below, for such calculations the bulk composition must be provided in terms of the full system - it is not sufficient here (unlike in normal calculations) to not consider SiO2 and H2O in the bulk composition, thus having q and H2O in excess..

> starting at the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :
```

> hitting return here means all phases are included in the calculations

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

find minimum Gibbs energy assemblage for a bulk composition ? yes
```

> The dogmin calculations were set up via a script in the datafile

```
max variance of equilibria to be looked at:
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
```

```
      n = n-variant
variance : 4
```

Note here that the wording of this variance question is quite different. The reason is that THERMOCALC, in trying to find the assemblage of lowest Gibbs energy for the given bulk composition at the PT of interest, loops through ALL of the divariant, then all of the trivariant, and so on, up to the user's choice of the maximum variance assemblage to be considered - in this case, quadrivariant

```
specification of PT window:
P range over which equilibria to be calculated
P window: P low,high : 9
T range over which equilibria to be calculated
T window: T low,high :  565 650
T window : 565 <-> 650°C :T interval : 5
```

The calculations are to be done at 9 kbar and 565°C to 650°C, at 5° intervals

```
use bulk compositions specified in datafile for pseudosection ? yes
composition (from script)
   H2O  SiO2 Al2O3   MgO    FeO    K2O
 22.58 45.16 13.51  5.87   8.80   4.07
```

This bulk composition is just the usual bulk composition but with H_2O and SiO_2 added. Care is needed to include sufficient of these so that all the assemblages of interest do indeed have q and H_2O in excess. (This can be done most easily, prior to setting the script dogmin, by adding H_2O and SiO_2 to the bulk for the most H_2O-rich assemblage - in this case the chl quadrivariant one - and ascertaining that the assemblage is seen).

In the datafile this was actually done with

```
        % [script to enter the bulk composition info]
        % --------------------------------------------------
        %             H2O SiO2   Al2O3    MgO     FeO     K2O
        setbulk yes    70  140   41.89  18.19   27.29   12.63
        % --------------------------------------------------
```

and THERMOCALC sums the numbers to a 100. Doing it like this means that, as the H_2O and SiO_2 are adjusted there is no chance of messing up the proportions of the other components.

There follows a more or less prodigious amount of output, as THERMOCALC loops through all the divariants, trivariants and quadrivariants. Then finally it produces a table

```
Gibbs energy minimisation info
```

P(kbar)	T(°C)	st	g	chl	bi	mu	ky	q	H2O	n	G	del
9.00	565.0	-	-	+	-	+	-	+	+	7	-844.74255	0.20262
9.00	570.0	-	-	+	-	+	-	+	+	7	-845.29150	0.17434
9.00	575.0	-	-	+	-	+	-	+	+	7	-845.84265	0.14605
9.00	580.0	-	+	+	-	+	-	+	+	8	-846.39636	0.00039
9.00	585.0	-	+	+	-	+	-	+	+	8	-846.95416	0.00273
9.00	590.0	-	+	+	-	+	-	+	+	8	-847.51611	0.00710
9.00	595.0	-	+	+	+	+	-	+	+	9	-848.08301	0.00104
9.00	600.0	-	+	+	+	+	-	+	+	9	-848.65564	0.00396
9.00	605.0	-	+	+	+	+	-	+	+	10	-849.23364	0.00858
9.00	610.0	-	+	+	+	+	-	+	+	10	-849.81677	0.00255
9.00	615.0	+	+	-	+	+	-	+	+	10	-850.41107	0.00404
9.00	620.0	+	+	-	+	+	-	+	+	10	-851.01007	0.00300
9.00	625.0	+	+	-	+	+	-	+	+	10	-851.61127	0.00203
9.00	630.0	+	+	-	+	+	-	+	+	11	-852.21454	0.00111
9.00	635.0	+	+	-	+	+	-	+	+	10	-852.81989	0.00024
9.00	640.0	-	+	-	+	+	+	+	+	10	-853.42798	0.00057
9.00	645.0	-	+	-	+	+	+	+	+	10	-854.03827	0.00133
9.00	650.0	-	+	-	+	+	+	+	+	10	-854.65063	0.00203

```
(Use these results at your own risk!)
```

Each row gives the assemblage with the lowest Gibbs energy at that PT. The n column gives the number of assemblages at that PT which are seen by the bulk composition, and therefore the number of Gibbs energies compared. The G column is the Gibbs energy of this assemblage, and the del column gives by how much this Gibbs energy is the smallest. If this number is very small, say < 10^-4, then it is *possible* that the identification of the most stable assemblage is incorrect. It is for this reason that the warning is given - and also because it is always possible for THERMOCALC to have not actually been able to calculate the assemblage with the lowest Gibbs energy, for example for starting guess reasons.

To illustrate the form of the output which is provided, prior to this table of stable assemblages being given, the results for the chl quadrivariant are shown next

```
<=====================================================>
phases : chl, (mu, q, fluid) or [st,g,bi,ky]
reactions : |X|X


-----------------------------------------------------------------
 P(kbar)       T(°C)    x(chl)    y(chl)     x(mu)     y(mu)
    9.00       565.0    0.5751    0.5477    0.8008    0.8008

  mode       chl        mu         q        H2O           G
          0.3433    0.5051    0.1137   0.03791  -844.74255
```

The only difference between this and normal output is that the Gibbs energy of the assemblage
is given after the modal information

```
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(mu)     y(mu)
   9.00       570.0    0.5751    0.5486    0.8001    0.8001

  mode        chl        mu         q        H2O         G
       0.3432    0.5052    0.1137   0.03791  -845.29150
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(mu)     y(mu)
   9.00       575.0    0.5751    0.5495    0.7995    0.7995

  mode        chl        mu         q        H2O         G
       0.3432    0.5052    0.1137   0.03791  -845.84265
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(mu)     y(mu)
   9.00       580.0    0.5751    0.5505    0.7988    0.7989

  mode        chl        mu         q        H2O         G
       0.3431    0.5053    0.1137   0.03791  -846.39594
------------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)    y(chl)     x(mu)     y(mu)
   9.00       585.0    0.5751    0.5514    0.7981    0.7983

  mode        chl        mu         q        H2O         G
       0.3431    0.5053    0.1137   0.03791  -846.95142
```

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Annotated THERMOCALC logfiles

Tx pseudosection

We now show how to generate a Tx pseudosection, for a bulk composition *line* entered into the datafile with the script:

```
%  [script to enter the bulk composition info]
%  --------------------------------------------------
%              Al2O3      MgO      FeO      K2O
setbulk        41.89        0    45.48    12.63
setbulk yes    41.89    45.48        0    12.63    50
%  --------------------------------------------------
```

This line was generated from the bulk composition used in the PT pseusosection calculations, which was

```
setbulk yes    41.89   18.19   27.29   12.63
```

by adding together the 18.19 and the 27.29, making 45.48, and using this for FeO in one bulk composition, with MgO zero, and vice versa for the other bulk composition. So the bulk composition line runs through the bulk composition of the PT pseudosection examples, from the pure FeO to the pure MgO subsystems.

This is the bulk composition line used for the Tx pseudosection discussed in the body of the paper. The diagram will be built up line by line and point by point, first locating the univariant curve for the staurolite isograd reaction in AFM. Only part of this reaction will be "seen" by our bulk composition line because the compositions of the phases in equilibrium at the reaction change along the reaction line. Various constructional features of the Tx pseudosection we wish to calculate are shown in the following figure
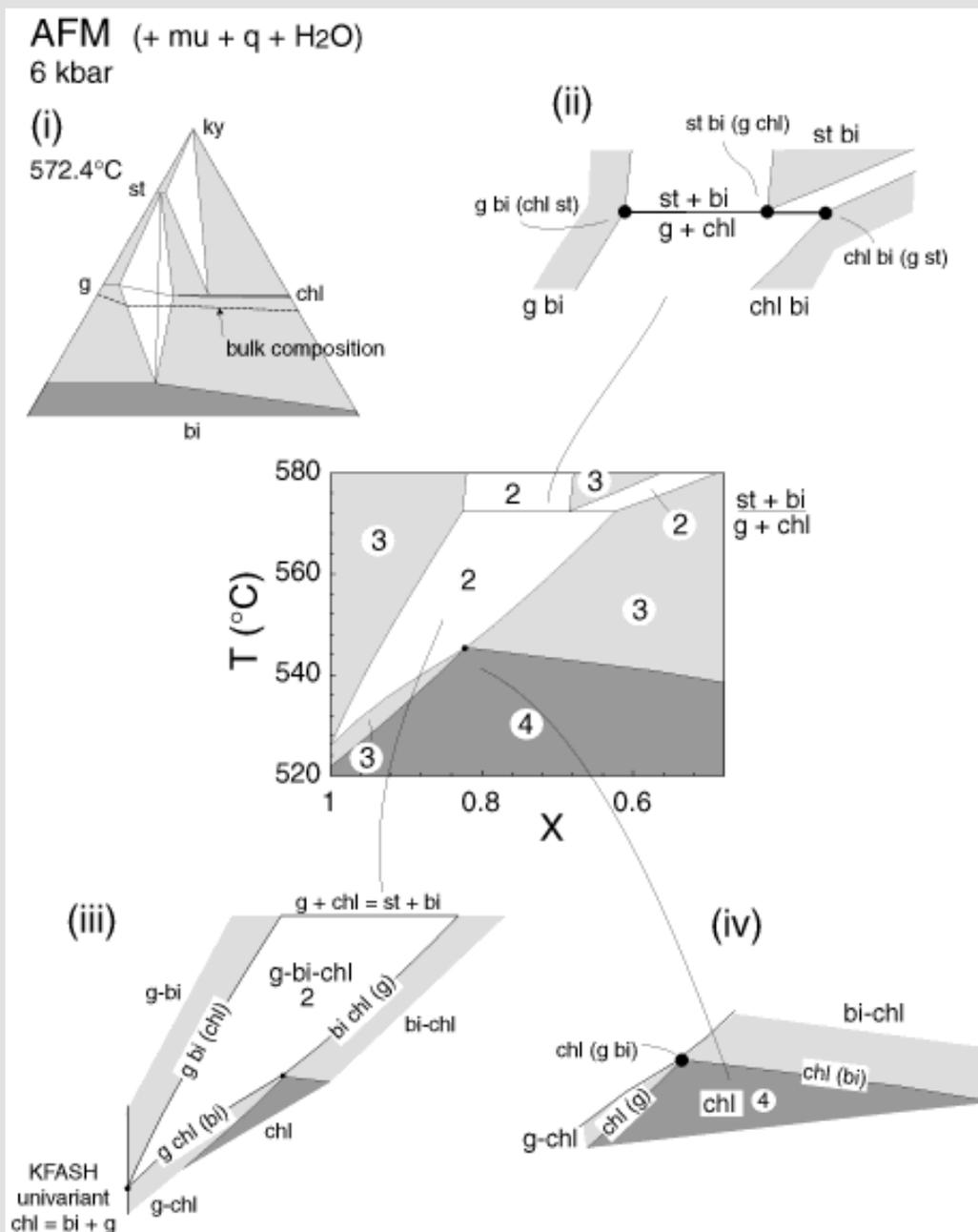
The labelling of points and lines in this figure are as in the PT pseudosection calculations, with the phases involved in the lower variance assemblage, with the phase(s) in brackets being those that have gone to zero (in going from the lower to the higher variance assemblage) at the point or line. So, in (i) in the figure, the point which is the low P end of the univariant, is denoted bi chl (st g) because the univariant assemblage is g + chl + bi + st, and, at the point, going into the trivariant, the modes of st and g are zero.

Note that on such diagrams the variance changes across lines (but not univariant lines) can only be by one, and that the maximum variance change across a point can only be by two.

```
THERMOCALC v2.5, © Roger Powell and Tim Holland running at 17.18 on Fri 6 Dec,1996
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)

calculation type :
```

```
      0 = table of thermodynamic data of end-members
      1 = phase diagram calculations
      2 = average pressure-temperature calculations
      3 = calculations on all reactions between end-members
      4 = list end-member names and compositions
control code  : 1
```

means do mode 1 phase diagram calculations

```
data filename : suffix to "th d" : st
```

filename to use is th dst

```
reading phase info from this file ...
st  ctd  cd  g  chl  bi  mu  and  ky  sill  ksp  q  H2O

log output will be found in "th log" (from prefs)
output will be found in the file, "th ost" (from prefs)
(thermodynamic dataset produced at 16.53 on Sat 20 Apr, 1996)
output will be found in the file, "th math" (from prefs)

phases ignored this run: ksp and sill ctd cd  (from script)
st  g  chl  bi  mu  ky  q  H2O
which phases :  omit ky
```

this time we want to calculate the ky-absent reaction

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 1

read in bulk compositions and
generate pseudosection information for them ? yes
```

this and the following black yeses were provided in scripts; this one for example by having "pseudosection yes" in the datafile

```
calculate trivariant points on univariants ? yes
you may set zero modal proportions, from:st g chl bi mu q H2O
which to set : (nothing input)
```

the yes here comes from the script "zeromodeiso yes", but having hit return at the "which to set" prompt, no

modes will be set...

```
equilibia now effectively univariant (eg is a line in PT)
```

...so the variance of the equilibrium is unchanged

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

specification of PT window:

use P window given in datafile ? yes
P window : 6.0 kbar (from script)
T window within which reactions expected to lie
T window: T low,high : (nothing input)
```

P = 6 kbar was set with a "setPwindow 6 6" script, and the T window is the default one set by a script in the datafile, activated as nothing was input at this prompt (by hitting return).

```
use bulk compositions specified in datafile for pseudosection ? yes

select a bulk composition range within the range specified ? yes

making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : (nothing input)
```

as nothing was input at this prompt (by hitting return), the whole composition range (denoted 0 <-> 1) is used.

```
how many increments (max is 100) : (nothing input)
```

as nothing was input at this prompt (by hitting return), the maximum number of intervals (100) is used.

```
composition
pos        1    11    21    31    41    51    61    71    81    91   101    (in this
range)
prop       0 0.100 0.200 0.300 0.400 0.500 0.600 0.700 0.800 0.900 1.000    (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO     0  4.55  9.10 13.64 18.19 22.74 27.29 31.84 36.38 40.93 45.48
   FeO 45.48 40.93 36.38 31.84 27.29 22.74 18.19 13.64  9.10  4.55     0
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
```

In this table, the compositions in the composition range are written out. In any output, the proportions are always given in absolute terms between 0 and 1. However, if an integer position is given, they are given in terms of the local range (as provided in the "start and finish proportions" prompt).

```
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions : |XX|X|X|XXX|XX
 P(kbar)      T(°C)     x(st)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    6.00      572.3    0.9366    0.9109    0.6039    0.5929    0.6378    0.4169    0.8118
```

```
0.8602
         19g + 33chl + 72mu = 10st + 72bi + 115q + 112H2O
```

The univariant occurs as a horizontal line on a T-x pseudosection

The following gives the entry and exit modes of the "seen" part of the univariant, for each of the bulk compositions in the composition line. At this end of the "seen" part, both the st and the chl modes are going to zero along the line, so the line terminates at the g+bi trivariant, at a point that can be referred to as g bi (chl st).

mode	st	g	chl	bi	mu
0.180		0.3822	0.0113	0.2027	0.4038
	0.0074	0.3778		0.2191	0.3956
0.190		0.3627	0.0332	0.1978	0.4063
	0.0218	0.3500		0.2461	0.3822
0.200		0.3433	0.0550	0.1930	0.4087
	0.0362	0.3221		0.2730	0.3687
0.210		0.3238	0.0769	0.1881	0.4111
	0.0505	0.2942		0.3000	0.3552
0.220		0.3044	0.0988	0.1833	0.4136
	0.0649	0.2664		0.3270	0.3417
0.230		0.2849	0.1207	0.1784	0.4160
	0.0793	0.2385		0.3539	0.3282
0.240		0.2655	0.1425	0.1736	0.4184
	0.0937	0.2107		0.3809	0.3148
0.250		0.2460	0.1644	0.1687	0.4208
	0.1080	0.1828		0.4079	0.3013
0.260		0.2266	0.1863	0.1639	0.4233
	0.1224	0.1550		0.4348	0.2878
0.270		0.2072	0.2081	0.1590	0.4257
	0.1368	0.1271		0.4618	0.2743
0.280		0.1877	0.2300	0.1541	0.4281
	0.1512	0.0992		0.4887	0.2608
0.290		0.1683	0.2519	0.1493	0.4306
	0.1656	0.0714		0.5157	0.2473
0.300		0.1488	0.2738	0.1444	0.4330
	0.1799	0.0435		0.5427	0.2339
0.310		0.1294	0.2956	0.1396	0.4354
	0.1943	0.0157		0.5696	0.2204
0.320		0.1099	0.3175	0.1347	0.4378
	0.1879		0.0317	0.5505	0.2299

Here, the exit assemblage has changed (between 0.31 and 0.32) - from the st+g+bi divariant to the st+chl+bi divariant, indicating that the st+bi trivariant terminates to lower temperature on the univariant line.

0.330		0.0905	0.3394	0.1299	0.4403
	0.1546		0.1041	0.4721	0.2691
0.340		0.0710	0.3613	0.1250	0.4427
	0.1214		0.1765	0.3937	0.3083
0.350		0.0516	0.3831	0.1201	0.4451
	0.0882		0.2489	0.3153	0.3475
0.360		0.0322	0.4050	0.1153	0.4476

```
        0.0550              0.3214   0.2369   0.3867
 0.370               0.0127  0.4269   0.1104   0.4500
        0.0217              0.3938   0.1585   0.4259
```

At this end of the "seen" part, both the g and the st modes are going to zero along the line, so the line terminates at the bi+chl trivariant, at a point that can be referred to as bi chl (g st).

```
more phase diagram calculations ? yes
```

Having determined the position of the horizontal line which is the univariant reaction, a number of points that can be calculated have been identified, we look at the bi chl (g st) point where the univariant terminates at the bi+chl trivariant.

To calculate the bi chl (g st) point, it is necessary to realise that THERMOCALC is not able (yet!) to calculate where an equilibrium is along a composition line. The point we are interested in can be thought of as a line in PTx. We determine where it is in Tx at 6 kbars by determining the PT at each x, and interpolating in Tx to get their values at 6 kbars. We can home in on the required conditions by specifying decreasing size x ranges, as we will do below.

starting with the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit ky
fluid is in excess (from script)

use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 1

read in bulk compositions and
generate pseudosection information for them ? yes

calculate trivariant points on univariants ? yes
you may set zero modal proportions, from:st g chl bi mu q H2O
which to set :   st g
```

Setting the modes of st and g to zero, means that we can now calculate the position of the bi chl (g st) point

```
equilibia now effectively invariant (eg is a point in PT)

specification of PT window:

use P window given in datafile ? yes
P window : 6.00 kbar (from script)
T window within which invariant points expected to lie
T window: T low,high : (nothing input)
P(low) must be less than P(high) : try again
P low,high :  4 8
```

P = 6 kbars is set as a script. However in this context, we have to calculate the PT points at a series of x values, so THERMOCALC flags the difficulty, and, via the "try again", a P range can be input. The choice should be one that straddles our 6 kbars value. It should be a large range if the point changes PT quickly as bulk composition changes; here a small range is sufficient

```
use bulk compositions specified in datafile for pseudosection ? yes

select a bulk composition range within the range specified ? yes
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : (nothing input)
```

as nothing was input at this prompt (by hitting return), the whole composition range (denoted 0 <-> 1) is used.

```
how many increments (max is 100) : 10
```

It is often better to use a coarse range to locate the point approximately, then to run the equilibrium again in a much smaller range, once its approximate position is known

```
composition
pos        1      2      3      4      5      6      7      8      9     10     11    (in this
range)
prop       0 0.100 0.200 0.300 0.400 0.500 0.600 0.700 0.800 0.900 1.000    (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO     0  4.55  9.10 13.64 18.19 22.74 27.29 31.84 36.38 40.93 45.48
   FeO 45.48 40.93 36.38 31.84 27.29 22.74 18.19 13.64  9.10  4.55     0
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
<=================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions : |XX|X|X|XXX|XX


70-------------------------------------------------------------------

 P(kbar)      T(°C)     x(st)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    4.04      541.1    0.9761    0.9643    0.7874    0.6077    0.8144    0.4474    0.9126
0.8785

  mode        st         g        chl        bi        mu
 0.200         0         0    0.4242    0.1413    0.4346
-------------------------------------------------------------------
```

```
 P(kbar)     T(°C)      x(st)      x(g)     x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    5.07     558.3     0.9568    0.9375    0.6830    0.5998    0.7159    0.4314    0.8589
0.8689

   mode        st         g        chl        bi        mu
 0.300         0         0     0.4331    0.1233    0.4435
------------------------------------------------------------
 P(kbar)     T(°C)      x(st)      x(g)     x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    6.31     576.8     0.9292    0.9014    0.5797    0.5906    0.6134    0.4120    0.7962
0.8573

   mode        st         g        chl        bi        mu
 0.400         0         0     0.4439    0.1018    0.4543
```

The calculated PT as gone from below 6 kbars to above 6 kbars between x = 0.3 and 0.4. So this can be used as the range in the next run

```
------------------------------------------------------------
 P(kbar)     T(°C)      x(st)      x(g)     x(chl)    y(chl)     x(bi)     y(bi)     x(mu)
y(mu)
    7.82     597.1     0.8889    0.8518    0.4769    0.5798    0.5071    0.3884    0.7218
0.8427

   mode        st         g        chl        bi        mu
 0.500         0         0     0.4570   0.07569    0.4674
77777
more phase diagram calculations ? yes

more phase diagram calculations ? no
all done ? yes
```

going round again, with the same equilibrium (so doing the run exactly the same as in the above), but now with a smaller range

missing out the first part of the log, and starting with the "start and finish proportions" prompt

```
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range :  0.3 0.4
how many increments (max is 100) : 10
composition
pos           1     2     3     4     5     6     7     8     9    10    11   (in this
range)
prop   0.300 0.310 0.320 0.330 0.340 0.350 0.360 0.370 0.380 0.390 0.400   (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO 13.64 14.10 14.55 15.01 15.46 15.92 16.37 16.83 17.28 17.74 18.19
   FeO 31.84 31.38 30.93 30.47 30.02 29.56 29.11 28.65 28.20 27.74 27.29
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
<==================================================>
```

```
phases : st, g, chl, bi, (mu, q, fluid)
reactions : |XX|X|X|XXX|XX

-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.07     558.3    0.9568    0.9375    0.6830    0.5998    0.7159    0.4314    0.8589
0.8689

   mode        st         g        chl        bi        mu
 0.300         0         0    0.4331    0.1233    0.4435
-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.19     560.1    0.9545    0.9343    0.6727    0.5989    0.7058    0.4296    0.8530
0.8679

   mode        st         g        chl        bi        mu
 0.310         0         0    0.4341    0.1213    0.4445
-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.30     561.9    0.9520    0.9311    0.6623    0.5981    0.6957    0.4278    0.8471
0.8668

   mode        st         g        chl        bi        mu
 0.320         0         0    0.4351    0.1193    0.4455
-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.42     563.7    0.9495    0.9278    0.6520    0.5972    0.6855    0.4260    0.8411
0.8657

   mode        st         g        chl        bi        mu
 0.330         0         0    0.4362    0.1173    0.4466
-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.54     565.5    0.9469    0.9243    0.6416    0.5963    0.6753    0.4241    0.8350
0.8645

   mode        st         g        chl        bi        mu
 0.340         0         0    0.4372    0.1152    0.4476
-------------------------------------------------------------------
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
y(mu)
    5.66     567.4    0.9443    0.9208    0.6313    0.5954    0.6651    0.4222    0.8288
0.8634

   mode        st         g        chl        bi        mu
 0.350         0         0    0.4383    0.1131    0.4487
reactions : |XX|X|X|XXX|XX
 P(kbar)     T(°C)     x(st)      x(g)     x(chl)    y(chl)     x(bi)      y(bi)     x(mu)
```

```
y(mu)
     5.79       569.2     0.9415     0.9172     0.6209     0.5945     0.6548     0.4202     0.8225
0.8622

   mode        st          g         chl        bi         mu
  0.360        0           0       0.4393     0.1109     0.4497
------------------------------------------------------------------------
 P(kbar)     T(°C)      x(st)       x(g)      x(chl)     y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     5.92       571.1     0.9386     0.9134     0.6106     0.5935     0.6445     0.4182     0.8160
0.8610

   mode        st          g         chl        bi         mu
  0.370        0           0       0.4404     0.1087     0.4508
------------------------------------------------------------------------
 P(kbar)     T(°C)      x(st)       x(g)      x(chl)     y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     6.05       573.0     0.9356     0.9095     0.6003     0.5926     0.6342     0.4162     0.8095
0.8598

   mode        st          g         chl        bi         mu
  0.380        0           0       0.4416     0.1065     0.4520
```

The Tx of the bi chl (g st) point is therefore about 572°C at x = 0.376. If necessary, THERMOCALC can be run again to get the position of the point more accurately

```
------------------------------------------------------------------------
 P(kbar)     T(°C)      x(st)       x(g)      x(chl)     y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     6.18       574.9     0.9325     0.9055     0.5900     0.5916     0.6238     0.4141     0.8029
0.8586

   mode        st          g         chl        bi         mu
  0.390        0           0       0.4427     0.1042     0.4531
------------------------------------------------------------------------
 P(kbar)     T(°C)      x(st)       x(g)      x(chl)     y(chl)     x(bi)      y(bi)      x(mu)
y(mu)
     6.31       576.8     0.9292     0.9014     0.5797     0.5906     0.6134     0.4120     0.7962
0.8573

   mode        st          g         chl        bi         mu
  0.400        0           0       0.4439     0.1018     0.4543

more phase diagram calculations ? yes
```

Running down T from the point just calculated is the bi chl (g) line separating the bi+chl+g divariant from the bi+chl trivariant. This is calculated now.

The bi chl (g) line can be calculated using the bi+chl+g divariant and setting the mode of g to

zero.

> starting at the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit st ky
```

> so that we are looking at the bi+chl+g divariant

```
fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
      0 = invariant
      1 = univariant
      2 = divariant
      3 = trivariant
      ...
      n = n-variant
variance : 2

read in bulk compositions and
generate pseudosection information for them ? yes

set mode isopleths ? yes

set modes to zero (to find edges/corners of fields ? yes
you may set zero modal proportions, from:g chl bi mu q H2O
which to set : g
```

> to look at the bi chl (g) line

```
equilibia now effectively univariant (eg is a line in PT)

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

specification of PT window:

use P window given in datafile ? yes
P window : 6.00 kbar (from script)
T window within which reactions expected to lie
T window: T low,high : (nothing input)
```

> so using P = 6 kabrs and the default T range

```
use bulk compositions specified in datafile for pseudosection ? yes

select a bulk composition range within the range specified ? yes
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : (nothing input)
```

> as nothing was input at this prompt (by hitting return), the whole composition range (denoted 0 <-> 1) is used.

```
how many increments (max is 100) : 10
```

> using 10 increments

```
composition
pos            1      2      3      4      5      6      7      8      9     10     11    (in this
range)
prop          0  0.100  0.200  0.300  0.400  0.500  0.600  0.700  0.800  0.900  1.000    (of
overall range)
 Al2O3 41.89  41.89  41.89  41.89  41.89  41.89  41.89  41.89  41.89  41.89  41.89
   MgO     0   4.55   9.10  13.64  18.19  22.74  27.29  31.84  36.38  40.93  45.48
   FeO 45.48  40.93  36.38  31.84  27.29  22.74  18.19  13.64   9.10   4.55      0
   K2O 12.63  12.63  12.63  12.63  12.63  12.63  12.63  12.63  12.63  12.63  12.63
<==================================================>
phases : g, chl, bi, (mu, q, fluid)
reactions :  |X|X|XXX|XX
```

> The following defines the Tx line which is bi chl (g). Note that, bewteen x = 0.1 and 0.2, the mode of bi goes to zero, suggesting that here a chl quadrivariant meets the bi+chl+g divariant.

```
77-------------------------------------------------------------------

 P(kbar)      T(°C)     x(g)    x(chl)    y(chl)    x(bi)     y(bi)     x(mu)     y(mu)
    6.00      547.8    0.9633   0.7863    0.5489   0.8089    0.3466    0.9139    0.8095

  mode         g        chl       bi        mu
 0.200         0      0.4890   0.01164   0.4994
-------------------------------------------------------------------
 P(kbar)      T(°C)     x(g)    x(chl)    y(chl)    x(bi)     y(bi)     x(mu)     y(mu)
    6.00      561.0    0.9368   0.6823    0.5730   0.7123    0.3844    0.8598    0.8386

  mode         g        chl       bi        mu
 0.300         0      0.4620   0.06564   0.4724
-------------------------------------------------------------------
 P(kbar)      T(°C)     x(g)    x(chl)    y(chl)    x(bi)     y(bi)     x(mu)     y(mu)
    6.00      576.1    0.9017   0.5800    0.5993   0.6148    0.4276    0.7958    0.8667

  mode         g        chl       bi        mu
 0.400         0      0.4347   0.1201    0.4451
-------------------------------------------------------------------
 P(kbar)      T(°C)     x(g)    x(chl)    y(chl)    x(bi)     y(bi)     x(mu)     y(mu)
    6.00      593.8    0.8542   0.4793    0.6286   0.5161    0.4775    0.7192    0.8936

  mode         g        chl       bi        mu
 0.500         0      0.4067   0.1763    0.4171
-------------------------------------------------------------------
 P(kbar)      T(°C)     x(g)    x(chl)    y(chl)    x(bi)     y(bi)     x(mu)     y(mu)
    6.00      614.8    0.7881   0.3800    0.6614   0.4159    0.5353    0.6266    0.9187
```

```
  mode          g          chl        bi          mu
 0.600          0     0.3770     0.2355     0.3874
------------------------------------------------------------
 P(kbar)      T(°C)        x(g)     x(chl)     y(chl)      x(bi)      y(bi)      x(mu)      y(mu)
    6.00      640.3     0.6928     0.2820     0.6984     0.3141     0.6024     0.5137     0.9413

  mode          g          chl        bi          mu
 0.700          0     0.3447     0.3001     0.3551
------------------------------------------------------------
 P(kbar)      T(°C)        x(g)     x(chl)     y(chl)      x(bi)      y(bi)      x(mu)      y(mu)
    6.00      671.9     0.5510     0.1855     0.7400     0.2105     0.6795     0.3748     0.9608

  mode          g          chl        bi          mu
 0.800          0     0.3085     0.3725     0.3189
------------------------------------------------------------
 P(kbar)      T(°C)        x(g)     x(chl)     y(chl)      x(bi)      y(bi)      x(mu)      y(mu)
    6.00      711.7     0.3341    0.09116     0.7862     0.1055     0.7644     0.2047     0.9763

  mode          g          chl        bi          mu
 0.900          0     0.2674     0.4548     0.2778
------------------------------------------------------------
 P(kbar)      T(°C)        x(g)     x(chl)     y(chl)      x(bi)      y(bi)      x(mu)      y(mu)
    6.00      762.1 1.265e-7  2.753e-8     0.8349  3.255e-8     0.8491 6.862e-8     0.9873

  mode          g          chl        bi          mu
 1.000          0     0.2228     0.5441     0.2332

more phase diagram calculations ? yes
```

The above suggest that the chl quadrivariant meets the bi+chl+g divariant, which will occur at a point that can be denoted chl (bi g). This is calculated next.

The calculation of the chl (bi g) point involves the same logic as involved in calculating the bi chl (g st) point above

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit st ky
fluid is in excess (from script)

use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
```

```
variance : 2
```

looking at the divariant

```
read in bulk compositions and generate pseudosection information for them ? yes
set mode isopleths ? yes

set modes to zero (to find edges/corners of fields ? yes
you may set zero modal proportions, from:g chl bi mu q H2O
which to set :   g bi
```

so looking at the chl (g bi) point

```
equilibia now effectively invariant (eg is a point in PT)

specification of PT window:

use P window given in datafile ? yes
P window : 6.00 kbar (from script)
T window within which invariant points expected to lie
T window: T low,high : (nothing input)
P(low) must be less than P(high) : try again
P low,high :   4 8
```

using P = 4 to 8 kbars, and the default T range

```
use bulk compositions specified in datafile for pseudosection ? yes

select a bulk composition range within the range specified ? yes
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : (nothing input)
```

as nothing was input at this prompt (by hitting return), the whole composition range (denoted 0 <-> 1) is used.

```
how many increments (max is 100) : 10
```

using 10 increments

```
composition
pos          1     2     3     4     5     6     7     8     9    10    11    (in this
range)
prop      0 0.100 0.200 0.300 0.400 0.500 0.600 0.700 0.800 0.900 1.000   (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO     0  4.55  9.10 13.64 18.19 22.74 27.29 31.84 36.38 40.93 45.48
   FeO 45.48 40.93 36.38 31.84 27.29 22.74 18.19 13.64  9.10  4.55     0
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
<======================================================>
phases : g, chl, bi, (mu, q, fluid)
reactions : |X|X|XXX|XX
```

```
1--------------------------------------------------------------

 P(kbar)      T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    5.46      534.7    0.9840    0.8926    0.5437    0.9059    0.3397    0.9601    0.8033

  mode          g        chl        bi        mu
 0.100          0    0.4948         0    0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    6.16      548.2    0.9632    0.7860    0.5441    0.8083    0.3388    0.9140    0.8031

  mode          g        chl        bi        mu
 0.200          0    0.4948         0    0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    6.98      563.2    0.9358    0.6803    0.5448    0.7074    0.3374    0.8602    0.8027

  mode          g        chl        bi        mu
 0.300          0    0.4948         0    0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    7.95      579.9    0.8990    0.5757    0.5457    0.6037    0.3352    0.7968    0.8021

  mode          g        chl        bi        mu
 0.400          0    0.4948         0    0.5052
777777
```

The chl (bi g) point occurs between x = 0.1 and 0.2, so this can be used (below) to home in on the point

```
more phase diagram calculations ? yes
```

going around again, to find the point more accurately

missing out the first part of the log, and starting with the "start and finish proportions" prompt

```
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range :  0.1 0.2
how many increments (max is 100) : 10
composition
pos         1     2     3     4     5     6     7     8     9    10    11   (in this
range)
prop   0.100 0.110 0.120 0.130 0.140 0.150 0.160 0.170 0.180 0.190 0.200   (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO  4.55  5.00  5.46  5.91  6.37  6.82  7.28  7.73  8.19  8.64  9.10
   FeO 40.93 40.48 40.02 39.57 39.11 38.66 38.20 37.75 37.29 36.84 36.38
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
<=============================================>
phases : g, chl, bi, (mu, q, fluid)
reactions : |X|X|XXX|XX

--------------------------------------------------------------
```

```
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.46      534.7     0.9840    0.8926    0.5437    0.9059     0.3397     0.9601     0.8033

 mode         g         chl        bi         mu
 0.100        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.52      536.0     0.9822    0.8819    0.5437    0.8963     0.3396     0.9558     0.8033

 mode         g         chl        bi         mu
 0.110        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.59      537.3     0.9803    0.8712    0.5438    0.8867     0.3396     0.9514     0.8033

 mode         g         chl        bi         mu
 0.120        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.66      538.6     0.9783    0.8606    0.5438    0.8770     0.3395     0.9470     0.8033

 mode         g         chl        bi         mu
 0.130        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.73      540.0     0.9763    0.8499    0.5438    0.8673     0.3394     0.9425     0.8033

 mode         g         chl        bi         mu
 0.140        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.80      541.3     0.9743    0.8392    0.5439    0.8575     0.3393     0.9379     0.8032

 mode         g         chl        bi         mu
 0.150        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.87      542.7     0.9722    0.8286    0.5439    0.8477     0.3392     0.9333     0.8032

 mode         g         chl        bi         mu
 0.160        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   5.94      544.0     0.9700    0.8179    0.5440    0.8379     0.3391     0.9286     0.8032

 mode         g         chl        bi         mu
 0.170        0       0.4948       0       0.5052
-------------------------------------------------------------------
P(kbar)      T(°C)       x(g)     x(chl)    y(chl)     x(bi)      y(bi)      x(mu)      y(mu)
   6.01      545.4     0.9678    0.8073    0.5440    0.8281     0.3390     0.9238     0.8031

 mode         g         chl        bi         mu
 0.180        0       0.4948       0       0.5052
```

so the chl (bi g) point is at about 546°C and x = 0.179

```
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.09      546.8    0.9655   0.7966   0.5441   0.8182   0.3389   0.9189   0.8031

   mode         g        chl        bi         mu
  0.190         0     0.4948         0     0.5052
-----------------------------------------------------------------
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.16      548.2    0.9632   0.7860   0.5441   0.8083   0.3388   0.9140   0.8031

   mode         g        chl        bi         mu
  0.200         0     0.4948         0     0.5052

more phase diagram calculations ? yes
```

Having determined the chl (g bi) point, it is straightforward to calculate the higher T boundary of the chl quadrivariant where it is bounded by the bi+chl trivariant, in other words the chl (bi) line.

The chl(bi) line is calculated via the bi+chl trivaraint, setting the mode of bi to zero.

starting with the "which phases" prompt

```
 st  g  chl  bi   mu  ky   q   H2O
which phases :   bi chl
fluid is in excess (from script)

use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance :  3

read in bulk compositions and
generate pseudosection information for them ? yes

set mode isopleths ? yes

set modes to zero (to find edges/corners of fields ? yes
you may set zero modal proportions, from:chl bi mu q H2O
which to set :  bi
```

so looking at the chl (bi) line

```
equilibia now effectively univariant (eg is a line in PT)

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

specification of PT window:

use P window given in datafile ? yes
P window : 6.00 kbar (from script)
T window within which reactions expected to lie
T window: T low,high : (nothing input)
```

using P = 6 kbars and the default T range

```
use bulk compositions specified in datafile for pseudosection ? yes

select a bulk composition range within the range specified ? yes
making a bulk composition range within the range specified,
start and finish proportions across bulk composition range : (nothing input)
```

as nothing was input at this prompt (by hitting return), the whole composition range (denoted 0 <-> 1) is used.

```
how many increments (max is 100) : 10
```

using 10 increments

```
composition
pos         1     2     3     4     5     6     7     8     9    10    11    (in this
range)
prop        0 0.100 0.200 0.300 0.400 0.500 0.600 0.700 0.800 0.900 1.000    (of
overall range)
 Al2O3 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89 41.89
   MgO     0  4.55  9.10 13.64 18.19 22.74 27.29 31.84 36.38 40.93 45.48
   FeO 45.48 40.93 36.38 31.84 27.29 22.74 18.19 13.64  9.10  4.55     0
   K2O 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63 12.63
<===================================================>
phases : chl, bi, (mu, q, fluid)
reactions : |XXX|X|X

-----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00      547.3    1.000    0.5547    1.000    0.3497    1.000    0.7962

  mode        chl        bi        mu
     0     0.4948        0     0.5052
-----------------------------------------------------------------
 P(kbar)      T(°C)    x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00      546.2    0.8925   0.5489   0.9052   0.3440   0.9600   0.8000

  mode        chl        bi        mu
```

```
 0.100   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     544.9   0.7861   0.5426   0.8086   0.3377   0.9141   0.8040

  mode      chl      bi       mu
 0.200   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     543.3   0.6809   0.5359   0.7104   0.3308   0.8608   0.8084

  mode      chl      bi       mu
 0.300   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     541.4   0.5770   0.5287   0.6106   0.3232   0.7984   0.8131

  mode      chl      bi       mu
 0.400   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     539.1   0.4748   0.5209   0.5095   0.3149   0.7245   0.8182

  mode      chl      bi       mu
 0.500   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     536.4   0.3744   0.5123   0.4074   0.3057   0.6357   0.8238

  mode      chl      bi       mu
 0.600   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     533.1   0.2763   0.5030   0.3047   0.2954   0.5275   0.8299

  mode      chl      bi       mu
 0.700   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     529.2   0.1808   0.4926   0.2020   0.2841   0.3930   0.8367

  mode      chl      bi       mu
 0.800   0.4948       0   0.5052
--------------------------------------------------------------
 P(kbar)      T(°C)   x(chl)   y(chl)    x(bi)    y(bi)    x(mu)    y(mu)
    6.00     524.7  0.08842   0.4812   0.1000   0.2714   0.2222   0.8442

  mode      chl      bi       mu
 0.900   0.4948       0   0.5052
1
more phase diagram calculations ? no
all done ? yes
```

In this way, moving along lines, calculating points, and so on, the whole of the Tx pseudosection can be built up...

Sometimes however it is difficult to get started in generating pseudosections, particularly in big systems. Gibbs energy minimisation facilities in THERMOCALC allow a start to be made. For T-x pseudosections, that approach would use one particular bulk composition for the calculation, say $x = 0.5$.

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Annotated THERMOCALC logfiles

Uncertainty calculations

Uncertainty calculations in phase diagram calculations are as simple as setting the script in the datafile

```
    calcsdnle yes
```

and then, whatever calculation is done, an uncertainty is generated. It is important to realise what exactly is involved in these uncertainties. They involve propagation *only* from the uncertainties on the thermodynamic data of the end-members of the phases, *not* from any uncertainty in the formulation of the activity-composition relationships of the phases. This means that the resulting uncertainties are almost certainly underestimates, sometimes seriously so. However, if uncertainties are already large with just the uncertainties on the thermodynamic data, they can only get larger with other uncertainties included. And *very crudely* a calculation that is insensitive to the thermodynamic data is likely to be insenstive to the activity- composition relationships. And vice versa.

THERMOCALC can do uncertainty propagation on individual calculations, but it cannot calculate the correlations between calculations. These correlations can be very significant as usually all the calculations will involve different but overlapping subsets of the same data. For example, thinking about a set of invariant points in a PT projection, THERMOCALC can calculate the uncertainties on the PT positions of the invariant points individually, but cannot tell, if a particular invariant point moves to higher P, say, where the other invariant points will move. Such considerations are critical for determining if a PT projection is close to changing topology, within the uncertainties on the thermodynamic data. Such determinations are possible only very laboriously with THERMOCALC and are beyond the present discussion.

There follows some examples of THERMOCALC uncertainty output, not in the form of full log output, but just in terms of results. Note that the uncertainties are 1 sigma, and that, with the exception of the PT of invariant points, the correlations between the values are not given.

A PT invariant point

```
<======================================================>
phases : st, g, chl, bi, ky, (mu, q, fluid)
reactions :  |XXX|XX|XXX|XX
```

```
     P(kbar)        T(°C)        x(st)        x(g)     x(chl)     y(chl)        x(bi)        y(bi)        x(mu)
y(mu)
        10.0          622        0.819        0.772      0.362      0.565        0.385        0.356        0.620
0.822
sd       0.8            7       0.0202       0.0191     0.0258    0.00912       0.0250       0.0483       0.0253
0.0160
correlation between P and T = -0.133
```

A univariant line at fixed P - the staurolite isograd reaction

```
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions :  |XX|X|X|XXX|XX
     P(kbar)        T(°C)        x(st)        x(g)     x(chl)     y(chl)        x(bi)        y(bi)        x(mu)
y(mu)
         8.0          599        0.884        0.846      0.466      0.579        0.496        0.386        0.713
0.841
sd                    11       0.0237       0.0276     0.0483    0.00755       0.0477       0.0562       0.0406
0.0126
        17g + 34chl + 73mu = 10st + 73bi + 114q + 118H2O
```

The bi chl (st g) point in the PT pseudosection

```
 Al2O3    MgO    FeO    K2O
 41.89  18.19  27.29  12.63
<=====================================================>
phases : st, g, chl, bi, (mu, q, fluid)
reactions :  |XX|X|X|XXX|XX

--------------------------------------------------------------
     P(kbar)        T(°C)        x(st)        x(g)     x(chl)     y(chl)        x(bi)        y(bi)        x(mu)
y(mu)
         6.3          577        0.929        0.901      0.580      0.591        0.613        0.412        0.796
0.857
sd       0.9            6      0.00617      0.00427    0.00203    0.00899      0.00712       0.0496      0.00897
0.0152
correlation between P and T = 0.283

   mode          st          g        chl         bi         mu
                  0          0      0.444      0.102      0.454
sd                               0.00930     0.0186    0.00930
```

The chl (bi g) point in a PT pseudosection

```
 Al2O3    MgO    FeO    K2O
```

```
 41.89 18.19 27.29 12.63
<=================================================>
phases : g, chl, bi, (mu, q, fluid)
reactions : |X|X|XXX|XX


-----------------------------------------------------------------
   P(kbar)        T(°C)      x(g)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
      8.0          580     0.899     0.576     0.546     0.604     0.335     0.797     0.802
sd    0.6            6   0.00451   0.00146   0.00878   0.00743    0.0546   0.00896   0.00573
correlation between P and T = 0.129

   mode          g       chl        bi        mu
                 0     0.495         0     0.505
sd                         0                   0
```

The chl (bi) line in a Tx pseudosection

```
composition
pos         1     2     3      4    (in this range)
prop   0.200 0.400 0.600  0.800   (of overall range)
 Al2O3 41.89 41.89 41.89 41.89
   MgO  9.10 18.19 27.29 36.38
   FeO 36.38 27.29 18.19  9.10
   K2O 12.63 12.63 12.63 12.63
<=================================================>
phases : chl, bi, (mu, q, fluid)
reactions : |XXX|X|X


-----------------------------------------------------------------
   P(kbar)        T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
      6.0          545     0.786     0.543     0.809     0.338     0.914     0.804
sd                  12  0.000916    0.0114   0.00474    0.0554   0.00463   0.00746

   mode        chl        bi        mu
 0.200       0.495         0     0.505
sd             0                   0
-----------------------------------------------------------------
   P(kbar)        T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
      6.0          541     0.577     0.529     0.611     0.323     0.798     0.813
sd                  12   0.00161    0.0111   0.00726    0.0546   0.00932   0.00728

   mode        chl        bi        mu
 0.400       0.495         0     0.505
sd             0                   0
-----------------------------------------------------------------
   P(kbar)        T(°C)    x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
      6.0          536     0.374     0.512     0.407     0.306     0.636     0.824
sd                  11   0.00192    0.0108   0.00733    0.0535    0.0131   0.00707

   mode        chl        bi        mu
 0.600       0.495         0     0.505
```

```
sd                 0                         0
-----------------------------------------------------------------
    P(kbar)       T(°C)     x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
       6.0          529     0.181     0.493     0.202     0.284     0.393     0.837
sd                   11   0.00158    0.0105   0.00486    0.0521    0.0131   0.00684

   mode        chl        bi        mu
  0.800      0.495         0     0.505
sd                0                   0
```

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```
    P(kbar)       T(°C)     x(chl)    y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
       6.0          529     0.181     0.493     0.202     0.284     0.393     0.837
```

THERMOCALC datafile used in examples

The following is the datafile, th dst (DOS: thdst.txt) used in the log examples. Anything after a % on a line is treated as annotation by THERMOCALC, and is not read by it. Down to the first *, the activity-composition relationships etc of the phases (*phase definitions*) are formulated (as in datafile structure). Between the first and the second * are the scripts. Beyond the second * is storage space not read by THERMOCALC. So the datafile structure is:

```
        phase definitions
        *
        scripts
        *
        storage
```

These parts are dealt with in turn.

Phase definitions

```
% -------------------- KFMASH datafile ------------------------

st 2   mst      1    1      1  1 -1  1  4     %   a(mst) = (1 - x)^4
                check 0
       fst      1    1      0  1  1  1  4     %   a(fst) = x^4
                bulk  1 1   0  1  1  1
                check 1
       x(st) 0.92                            %   x = Fe/(Fe + Mg)

ctd 2 mctd      1    1      1  1 -1  1  1     %   a(mctd) = (1 - x)
                check 0
       fctd     1    1      0  1  1  1  1     %   a(fctd) = x
                bulk  1 1   0  1  1  1
                check 1
       x(ctd) 0.91                           %   x = Fe/(Fe + Mg)

cd 3   crd      1    2      1  1 -1  1  2     %   a(crd) = (1 - x)^2 *
                           1  1 -1  2  1     %              (1 - h)
       fcrd     1    2      0  1  1  1  2     %   a(fcrd) = x^2 *
                           1  1 -1  2  1     %                (1 - h)
                bulk  1 1   0  1  1  1
       hcrd     1    2      1  1 -1  1  2     %   a(crd) = (1 - x)^2 *
```

```
                          0   1   1   2   1       %                h
                 bulk  1 1   0   1   1   2
        x(cd) 0.45                                 %  x = Fe/(Fe + Mg)
        h(cd) 0.7                                  %  h = H2O pfu

g 2     py      1    1      1   1  -1   1   3      %  a(py) = (1 - x)^3
                 check 0
        alm     1    1      0   1   1   1   3      %  a(alm) = x^3
                 bulk  1 1      0   1   1   1
                 check 1
        x(g) 0.9                                   %  x = Fe/(Fe + Mg)

chl 3 clin    16      3      1   1  -1   1   5      %  a(clin) = 16 (1 - x)^5 *
                             1   1  -1   2   2      %           (1 - y)^2 *
                             0   1   1   2   2      %            y^2
                 check 0 1/2
        daph    16      3      0   1   1   1   5      %  a(daph) = 16 x^5 *
                             1   1  -1   2   2      %           (1 - y)^2 *
                             0   1   1   2   2      %            y^2
                 bulk 1/5 2   0   1   2   1
                             3   1  -1   2
                 check 1 1/2
        ames    1      2      1   1  -1   1   4      %  a(ames) = (1 - x)^4 *
                             0   1   1   2   4      %             y^4
                 bulk  1 1  -1   1   2   2
                 check 0 1
        x(chl) 0.5                                 %  x = Fe/(Fe + Mg)
        y(chl) 0.6                                 %  y = oct Al/2

bi 3  phl    1/4   4      1   1  -1   1   3      %  a(phl) = 1/4 (1 - x)^3 *
                             2   1  -1   2   2      %           (2 - y)^2 *
                             1   1   1   2   1      %           (1 + y) *
                             1   1  -1   2   1      %           (1 - y)
                 check 0 0
        ann    1/4   4      0   1   1   1   3      %  a(ann) = 1/4 x^3 *
                             2   1  -1   2   2      %           (2 - y)^2 *
                             1   1   1   2   1      %           (1 + y) *
                             1   1  -1   2   1      %           (1 - y)
                 bulk 1/3 2 0   1   1   1
                             3   1  -1   2
                 check 1 0
        east   1/4   4      1   1  -1   1   2      %  a(east) = 1/4 (1 - x)^2 *
                             0   1   1   2   1      %            y *
                             1   1   1   2   2      %           (1 + y)^2 *
                             2   1  -1   2   1      %           (2 - y)
                 bulk  1 1  0   1   1   2
                 check 0 1
        x(bi) 0.5                                 %  x = Fe/(Fe + Mg)
        y(bi) 0.49                                %  y = oct Al
```

```
mu  3   mu      1/4   3         1  1  1  2  2      %  a(mu) = 1/4 (1 + y)^2 *
                                2  1 -1  2  1      %              (2 - y) *
                                0  1  1  2  1      %                 y
                check 0 1
        cel     1/4   4         1  1 -1  1  1      %  a(cel) = 1/4 (1 - x) *
                                1  1 -1  2  1      %               (1 - y) *
                                1  1  1  2  1      %               (1 + y) *
                                2  1 -1  2  2      %               (2 - y)^2
                bulk  1 2  1  1 -1  1
                           1  1 -1  2
                check 0 0
        fcel    1/4   4         0  1  1  1  1      %  a(fcel) = 1/4 x *
                                1  1 -1  2  1      %                (1 - y) *
                                1  1  1  2  1      %                (1 + y) *
                                2  1 -1  2  2      %                (2 - y)^2
                bulk  1 2  0  1  1  1
                           1  1 -1  2
                check 1 0
        x(mu) 0.75                              %  x = Fe/(Fe + Mg)
        y(mu) 0.95                              %  y = oct Al - 1

and ky sill q H2O                %  no solid solution phases
```

Scripts

There follows datafile script combinations for different calculations (these are to go between the stars in the datafile structure). The first batch was always included. In the following, the scripts involve either "yes" or "no", although in each case, "ask", could be used. With "ask", THERMOCALC will prompt you for the required behaviour.

One way to operate with THERMOCALC, is to have the various scripts which will be "yes" or "no" in a set of runs, all set to "ask", rather than as done below. Then, when running THERMOCALC, the corresponding prompts can be answered appropriately. RP finds that this can get confusing. He prefers to have the datafile open in a text editor - BBEdit (on the Mac) allows one do this (as it holds the file in RAM) - and to adjust the scripts as needed between runs or groups of runs, and use "yes" or "no" in the scripts. (His aim in running THERMOCALC is that as much as reasonably possible should be attainable by just hitting return, answering prompts: the scripts are used to make this possible).

Note that, in scripts, after the first word (keyword), there is an optional "yes", "no" or "ask". This includes those, like setproject below, that provide information. As in simple switches,

if the "yes", "no" or "ask"is omitted, "yes" is assumed.

Some general purpose scripts for the AFM calculations

```
moreprec yes                      % to output more precision on results
calcsdnle no                      % to calculate uncertainties

omit sill and ctd cd              % phases omitted in calculations

fluidpresent yes
fluidexcess yes                   % H2O in excess...
setexcess mu q                    % ... and mu, q: thus KFMASH -> AFM

setdefPwindow    1  14            % setting a default PT window
setdefTwindow  200 900

calctatp yes                      % to specify calculating T at fixed P
```

To be used when PT projection calculations are done (switching common scripts off)

```
project no
setiso no
pseudosection no
dogmin no
```

To be used when projections are to be done (otherwise "project no" used, and then setproject can be present, but won't be used). With just this (without the setproject script, or if the setproject script is of the form "setproject no ..."), then you are prompted for the projection plane to use. You are also prompted for the plane if there is a mismatch between the number of projection plane corners, or the number of components they are described with, and the numbers THERMOCALC thinks there should be.

```
project yes
```

To be used when projections are to be done (otherwise "project no" used, and then setproject can be present, but won't be used). This is the standard AFM projection plane as

used in the projection calculations.

```
project yes
% [script to enter the projection plane info]
% -------------------------------------------
setproject      A          1     0     0     0
setproject      F          0     0     1     0
setproject yes  M          0     1     0     0
% -------------------------------------------
```

To be included when isopleths to be calculated (otherwise "setiso no" used), for example in the isopleth example

```
setiso yes
```

To be included when a PT pseudosection is to be calculated. With just this (without the setbulk script, or if the setbulk script is of the form "setbulk no ..."), then you are prompted for the bulk composition to use. You are also prompted for the bulk composition if there is a mismatch between the number of components you have provided and the number THERMOCALC thinks there should be.

```
pseudosection yes
```

To be included when a PT pseudosection is to be calculated, and the bulk composition is as given. This particular composition is the one used for the PT pseudosection in the published paper, and in the PT pseudosection examples.

```
pseudosection ask
% [script to enter the bulk composition info]
% --------------------------------------------------
%             Al2O3    MgO     FeO    K2O
setbulk yes   41.89  18.19  27.29  12.63
% --------------------------------------------------
setmodeiso yes                              % allowing modes to be set
zeromodeiso yes                             % allowing zero modes to be set
```

To be included when a PT pseudosection is to be calculated, and the bulk composition line is as given. This particular composition line is the one used for the Tx pseudosection in the published paper, and in the [Tx pseudosection](#) examples; it runs through the bulk composition above.

```
% [script to enter the bulk composition info]
% -------------------------------------------------
%              Al2O3       MgO      FeO     K2O
setbulk        41.89         0    45.48   12.63
setbulk yes    41.89     45.48        0   12.63
% -------------------------------------------------
setmodeiso yes                                        % allowing modes to be set
zeromodeiso yes                                       % allowing zero modes to be set
```

To be included when a PT pseudosection is to be calculated, and the bulk composition line is as given; it runs through the bulk composition above and involves varying Al/(Fe+Mg) through above bulk

```
% [script to enter the bulk composition info]
% -------------------------------------------------
%              Al2O3      MgO      FeO      K2O
setbulk        12.63    29.90    44.84    12.63
setbulk yes    87.37     0.00     0.00    12.63
% -------------------------------------------------
setmodeiso yes                                        % allowing modes to be set
zeromodeiso yes                                       % allowing zero modes to be set
```

To be included when a Gibbs energy minimisation is to be done, and the bulk composition line is as given. This was used with the [Gibbs energy minimisation](#) example. The amount of H_2O and SiO_2 that needed to be added to the above bulk composition to make q and H_2O to always be in excess was found by trial and error.

```
% [script to enter the bulk composition info]
% -------------------------------------------------
%              H2O SiO2  Al2O3      MgO      FeO      K2O
setbulk yes     70  140  41.89    18.19    27.29    12.63
% -------------------------------------------------
dogmin yes
```

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KFMASH phases and end-members: abbreviations and formulae.

phase abbrev.	phase full name	end-member abbrev.	end-member full name	formula
mu	muscovite	mu	muscovite	$KAl_3Si_3O_{12}H_2$
		cel	celadonite	$KMgAlSi_4O_{12}H_2$
		fcel	Fe celadonite	$KFeAlSi_4O_{12}H_2$
bi	biotite	phl	phlogopite	$KMg_3AlSi_3O_{12}H_2$
		ann	annite	$KFe_3AlSi_3O_{12}H_2$
		east	eastonite	$KMg_2Al_3Si_2O_{12}H_2$
chl	chlorite	clin	clinochlore	$Mg_5Al_2Si_3O_{18}H_8$
		ames	amesite	$Mg_4Al_4Si_2O_{18}H_8$
		daph	daphnite	$Fe_5Al_2Si_3O_{18}H_8$
cd	cordierite	crd	cordierite	$Mg_2Al_4Si_5O_{18}$
		hcrd	hydrous cordierite	$Mg_2Al_4Si_5O_{19}H_2$
		fcrd	Fe cordierite	$Fe_2Al_4Si_5O_{18}$
ctd	chloritoid	mctd	Mg chloritoid	$MgAl_2SiO_7H_2$
		fctd	Fe chloritoid	$FeAl_2SiO_7H_2$
st	staurolite	mst	Mg staurolite	$Mg_4Al_{18}Si_{7.5}O_{48}H_4$
		fst	Fe staurolite	$Fe_4Al_{18}Si_{7.5}O_{48}H_4$
g	garnet	py	pyrope	$Mg_3Al_2Si_3O_{12}$
		alm	almandine	$Fe_3Al_2Si_3O_{12}$
		gr	grossular	$Ca_3Al_2Si_3O_{12}$
and	andalusite	and	andalusite	Al_2SiO_5
ky	kyanote	ky	kyanite	Al_2SiO_5
sill	sillimanite	sill	sillimanite	Al_2SiO_5
q	quartz	q	quartz	SiO_2
H_2O	fluid	H_2O	water fluid	H_2O

THERMOCALC output

Reaction coefficients

In writing reactions between solid solutions, it is possible for the range of reaction coefficient values to be very large; indeed it is possible in degenerate reactions for phases to have zero reaction coefficients.

THERMOCALC generates reaction coefficients which are not naturally normalised; they need to be multiplied up in some way to make them more easily understood.

Given that reaction coefficients can be identically zero (although THERMOCALC may not be able to establish this, because, for example, of rounding errors in the calculations), simply dividing through all of the reaction coefficients by the smallest one is not a sensible option.

The policy followed by THERMOCALC for each reaction is as follows (dealing with the absolute values of the coefficients):

- Determine"large", the largest reaction coefficient
- Any coefficient less than 10^{-7} of "large" is deemed to be identically zero, and is not mentioned in the reaction as written. Sometimes this is not a loose enough constraint, and phases whose coefficients are in fact identically zero, are nevertheless included in the reaction. These phases are removed from further consideration.
- Determine "small", the smallest of the remaining reaction coefficients which are 10^{-3} of "large".
- Coefficients larger than 10^{-3} of "large" are output as 10 times the reaction coefficient divided by "small": thus the smallest of these is output as10.
- Coefficients between 10^{-7} and 10^{-3} of "large" are output as 0 (and these may include phases which should not appear in the reaction because their reaction coefficients are identically zero)

This unfortunately has to be a bit technical because of the nature of the problem...

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Annotated THERMOCALC logfiles

Singularity example

It sometimes happens that when one looks along a PT univariant that something odd happens: one (or more) phases change sides on the reaction. Where this occurs is a singularity. They occur when phases become coplanar in the compatibility diagram being used. One does occur in our AFM example, in the [st] reaction that goes to higher pressure from the invariant point.

> starting with the "which phases" prompt

```
st  g  chl  bi  mu  ky  q  H2O
which phases :   omit st

fluid is in excess (from script)
use in excess phases specified in datafile ? yes
phases in excess: mu q  (from script)

variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
     3 = trivariant
     ...
     n = n-variant
variance : 1

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

specification of PT window:
P range over which T of reactions to be calculated
P window: P low,high :   9.5 12.5
T window within which reactions expected to lie
T window: T low,high : (nothing input)
P window :9.5 <-> 12.5 kbar :P interval : 0.25


<=====================================================>
phases : g, chl, bi, ky, (mu, q, fluid)
reactions : |XX|X|XXX|XX
 P(kbar)      T(°C)      x(g)    x(chl)   y(chl)     x(bi)     y(bi)     x(mu)     y(mu)
    9.50       618.2    0.7859   0.3798   0.5703    0.4037    0.3657    0.6369    0.8286
        10g + 323chl + 650mu = 650bi + 680ky + 624q + 1293H2O
```

> here the reaction is g + chl = bi + ky (just in terms of the AFM phases) - compare with the end of this listing. To properly understand the reaction coefficients, as they evolve along the reaction line below, it is

necessary to understand how THERMOCALC outputs reaction coefficients.

```
     9.75       620.3    0.7782     0.3704     0.5675     0.3933     0.3602     0.6280     0.8249
          10g + 400chl + 801mu = 801bi + 836ky + 768q + 1599H2O
    10.00       622.4    0.7705     0.3613     0.5648     0.3832     0.3548     0.6191     0.8212
          10g + 522chl + 1043mu = 1043bi + 1086ky + 999q + 2087H2O
    10.25       624.5    0.7626     0.3523     0.5620     0.3733     0.3495     0.6103     0.8174
          10g + 736chl + 1466mu = 1466bi + 1523ky + 1403q + 2943H2O
    10.50       626.5    0.7547     0.3436     0.5593     0.3636     0.3442     0.6015     0.8137
          10g + 1241chl + 2465mu = 2465bi + 2555ky + 2357q + 4963H2O
    10.75       628.5    0.7467     0.3350     0.5566     0.3541     0.3389     0.5927     0.8099
          0g + 10chl + 20mu = 20bi + 20ky + 19q + 40H2O
```

here, at 10.75 kbar, g is on the left side of the reaction with a tiny reaction coefficient ...

```
    11.00       630.4    0.7386     0.3267     0.5539     0.3448     0.3337     0.5840     0.8061
          10chl + 20mu = 0g + 20bi + 20ky + 19q + 40H2O
```

... whilst here, at 11 kbar, g is on the right side of the reaction with a tiny reaction coefficient.

This can be viewed as the reaction coefficient of g getting realtively smaller on the left side of the reaction with increasing P, going to zero, then getting relatively larger, but on the right side of the reaction.

So, garnet has changed sides on the reaction. This has occurred because chlorite has moved from being more magnesian to being more ferrous than the ky-bi tie line. There is in fact a singular reaction , ky+bi=chl, that emanates tangentially from a singular point on the univariant,where the reaction coefficient of g goes to zero, and runs up P. THERMOCALC is not able to calculate the position of singular reactions, although its ends can be inferred in the same way as here.

```
    11.25       632.3    0.7305     0.3185     0.5513     0.3357     0.3285     0.5754     0.8022
          1270chl + 2501mu = 10g + 2501bi + 2575ky + 2390q + 5078H2O
    11.50       634.2    0.7223     0.3106     0.5486     0.3268     0.3233     0.5668     0.7984
          771chl + 1515mu = 10g + 1515bi + 1555ky + 1447q + 3083H2O
    11.75       636.0    0.7140     0.3028     0.5459     0.3181     0.3182     0.5582     0.7945
          556chl + 1090mu = 10g + 1090bi + 1117ky + 1042q + 2225H2O
    12.00       637.8    0.7057     0.2951     0.5433     0.3096     0.3132     0.5497     0.7906
          437chl + 854mu = 10g + 854bi + 873ky + 817q + 1748H2O
    12.25       639.6    0.6973     0.2877     0.5406     0.3013     0.3082     0.5412     0.7866
          361chl + 704mu = 10g + 704bi + 717ky + 674q + 1444H2O
    12.50       641.3    0.6888     0.2803     0.5380     0.2931     0.3032     0.5327     0.7827
          308chl + 600mu = 10g + 600bi + 609ky + 574q + 1233H2O
```

while here the reaction is chl = g + bi + ky

```
more phase diagram calculations ? no
all done ? yes
```

singularity example