Calculating phase diagrams with THERMOCALC

These notes were developed by RP in or before 2001, for various THERMOCALC short courses and websites. My minor edits and annotations in *blue* reflect progress since then. - ECR Green, Nov 2019.

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The "background>introduction" and "background>calculating mineral equilibria" sections provide a necessary introduction to this section. We shall assume that an appropriate THER-MOCALC datafile has already been made for the model system of interest. [Don't worry about this...]

PT projections show the stable univariant and invariant equilibria for all of the composition space of the model system. Depending on whether univariants affect parts of the composition space that are petrologically interesting, PT projections may not be very interesting in themselves. Given that the compositions of the phases vary along univariants in PT projections, sometimes quickly, the parts of composition space that are affected by univariants may be difficult to gauge. With the exception of simple systems, PT projections can be almost impossible to use directly.

Pseudosections show the dependence of phase relationships of particular model system compositions on PT, so can be used to relate how particular rocks respond to changing metamorphic conditions. As a consequence they are often the most important phase diagrams to draw. Our interest in drawing PT projections is often only as an essential precursor to drawing pseudosections.

Compatibility diagrams show all the phase relationships for all compositions in the model system at the specified PT. As choosing phases to be "in excess" to reduce the model system to being effectively ternary—so that a triangular compatibility diagram can be drawn—may be difficult or impossible for the larger systems now being considered, compatibility diagrams are becoming less important.

Calculating PT projections

The constructional features of P–T projections, involving invariant¹ points and univariant lines, are generally familiar.

Getting THERMOCALC to calculate the lines and points for a P-T projection is simple a matter of specifying the phases involved, and the variance of the equilibria required. Generally it is best to do this with the phases for each invariant point in turn, calculating the position of the invariant point, and all the univariants around the point. Schreinemakers analysis at each point is then done, followed by the putting together of the invariant points to determine which are stable.

Depending on the model system, there be many or a very few stable invariant points. In NCFMASH for blueschists and eclogites there are over a hundred (ask Gisella Rebay who has calculated them!), whereas in NCKFMASH at upper amphibolite and granulite facies conditions there are only a few univariants and one invariant (see White *et al.* 2001). Nevertheless knowing the *PT* projection is a necessary step because it provides the overall stability framework of the

¹for an n component system, involving p phases, the variance v is equal to n-p+2, otherwise known as the phase rule. Invariant: v=0; univariant: v=1; divariant: v=2; and so on

phase equilibria, and, if any univariants are stable in the pseudosection, this gives an invaluable start to the construction of the pseudosection.

The annotated log files in the old web site (circa Powell et al., 1998) are a good place to look at this point (although things have changed a little bit since then). The simplicity of calculating an invariant (with TH KA1, a datafile with coding of the minerals in KFMASH²) can be seen from the following log file—user input is highlighted. An ellipsis at the end of a line signals that some output has been cut out. Where it says "(from script)", it means that the action was controlled by a datafile script; where it says "(nothing input)", it means that on the prompt for information return was hit, resulting in a default being used (in the case here, the PT window comes from the "setdefT window" and "setdefP window" scripts in the datafile).

```
reading phase info from this file ...
chl bi cd st ctd g mu ksp ky sill and q H20
which phases : bi st g chl ky
fluid in excess (from script)
phases in excess: mu q (from script)
variance of required equilibria :
    0 = invariant
    1 = univariant
    2 = divariant
    n = n-variant
variance: 0
specification of PT window:
PT window within which invariant points expected to lie
T low, high, P low, high: (nothing input)
<===========>>
phases : chl, bi, st, g, ky, (mu, q, fluid)
reactions : |XXXX|XX|XXX|XXX|--X
P(kbar)
            T(C)
                   x(chl)
                           y(chl)
                                    Q(chl)
                                              x(bi)
                                                       y(bi)
                                                               Q(bi)
                                                                        x(st)
                                                                                  x(g) \dots
   11.20
           639.6
                   0.3067
                           0.5534
                                    0.4465
                                             0.3495
                                                      0.2008
                                                              0.4348
                                                                       0.7462
                                                                                0.7244 ...
```

Note that output gives the composition of all the phases at the invariant as well as its PT. (It also gives the state of order of the chlorite and muscovite—the Q values). Compared to the figures in Powell $et\ al.\ (1998)$, this is a somewhat different result, being at about a kbar higher P, for several reasons: one is the more recent dataset used, the other is that chlorite and biotite are modelled using order-disorder. (Adding the script "calcsdnle yes" to the datafile and rerunning shows that this P has a 2σ uncertainty of about 1.5 kbar, so the difference is not considered to be a problem).

Running a univariant is almost as easy:

```
chl bi cd st ctd g mu ksp ky sill and q H2O which phases: bi chl st g fluid in excess (from script) phases in excess: mu q (from script)
```

 $^{^{2}}$ the datafile name organisation is given in a separate documentation file th ka1.txt was an axfile, which would today be called tc-ka1.txt or perhaps tc-KFMASH.txt.

```
variance of required equilibria:
    0 = invariant
    1 = univariant
    2 = divariant
    n = n-variant
variance: 1
specification of PT window:
P range over which T of reactions to be calculated
P window: P low, high: 4 12
T window within which reactions expected to lie
T window: T low, high: (nothing input)
P window :4 <-> 16 kbar :P interval : 2
<-----
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
P(kbar)
             T(C)
                                                                  Q(bi)
                                                                          x(st)
                    x(chl)
                             y(chl)
                                      Q(chl)
                                                x(bi)
                                                        y(bi)
                                                                                    x(g) ...
   4.00
            536.2
                    0.8803
                                      0.3276
                                                        0.6216
                                                               0.02812
                                                                          0.9822
                                                                                  0.9816 ...
                             0.6724
                                               0.9293
       22chl + 42g + 86mu = 86bi + 10st + 178g + 69H2O
   6.00
            579.4
                    0.6017
                             0.5981
                                      0.4018
                                               0.6663
                                                        0.4169
                                                                 0.2107
                                                                         0.9155
                                                                                  0.9111 ...
       31chl + 23g + 74mu = 74bi + 10st + 125q + 103H20
   8.00
            606.5
                    0.4608
                            0.5742
                                      0.4258
                                               0.5022
                                                        0.2861
                                                                 0.3649
                                                                         0.8552
                                                                                  0.8458 ...
       33chl + 17g + 68mu = 68bi + 10st + 102q + 112H20
                                                                          0.7900
                                                                                  0.7736 ...
   10.00
            628.0
                    0.3586
                             0.5598
                                      0.4401
                                               0.3990
                                                        0.2237
                                                                 0.4283
       33chl + 16g + 66mu = 66bi + 10st + 96q + 111H20
   12.00
            646.9
                    0.2750
                             0.5498
                                      0.4502
                                               0.3191
                                                        0.1888
                                                                 0.4289
                                                                          0.7148
                                                                                  0.6887 ...
       32chl + 17g + 65mu = 65bi + 10st + 96q + 108H20
```

The output gives the composition of the phases along the univariant as well as the T at each specified P. Note how the minerals change composition along the univariant, with x for the ferromagnesians becoming larger as P increases. The output also gives the balanced reaction (each mineral on on a one oxide basis) at each P.

Calculating along a stable univariant, 3 things can happen:

- 1. the univariant is cut off by a invariant, as happens in the above case with the invariant involving, additionally, kyanite (also calculated above). The relative stabilities have to be established with Schreinemakers analysis.
- 2. the univariant dies at an end-member system invariant, as would happen along the above calculated reaction at about 3.5 kbar, in the KFASH system. It then remains to be established whether the univariant survives to that point, or is cut off by an invarian. In this case, the latter is true, with a full-system invariant involving, additionally, chloritoid (at 4.2 kbar).
- 3. THERMOCALC fails to calculate the univariant beyond a certain point, but no end-member system invariant is being approached. This signals a failure of the non-linear equation solver in THERMOCALC. The usual resolution is to vary the starting guesses in the datafile, using ones that correspond to the values along the univariant that THERMOCALC could calculate.

Later in this file, some special cases and special tricks are outlined.

Calculating PT and Tx/Px pseudosections

Pseudosections involve the invariant and univariant equilibria they inherit from PT projections, as well as additional boundary lines and points. In a PT pseudosection these inherited equilibria are just those parts of the PT projection "seen" by the bulk composition being considered. In a Tx pseudosection these inherited equilibria occur as horizontal lines, spanning the range of bulk compositions that "sees" an equilibrium. The boundary lines and points separate fields of different variance; across lines the variance changes by one, and through points by two. The boundary points and lines can be most easily discussed with a new notation. Labelling is done in terms of the lower variance assemblage involved, with the names of phases with zero modes given in brackets. So for example in Fig. 1(iii), going from the g-chl-bi divariant field, through the point at 8 kbar and 580°C, into the chl quadrivariant field, the modes of bi and g both go to zero at the point. The point is therefore labelled "chl (bi g)". Similarly, in going down T at 10 kbar from the g-chl-bi divariant field into the g-chl trivariant field into the chl quadrivariant field, the two lines crossed are labelled "chl g (bi)" and "chl (g)".

The labelling of boundaries (and points) in terms of the phases whose mode(s) go to zero is shown in Figs 1 and 2. In THERMOCALC terminology such a boundary line is called "effectively" univariant (regardless of the variance of the fields) because, in terms of variables, the boundary is a line. The effective univariance³ comes from the the combining of the bulk composition with the equlibrium relationships.

In terms of a coherent view of pseudosection construction features, different rules appear to apply across univariants, with this being the one situation in which variance does not change by one (or, alternatively, the number of phase in the assemblage changing by one) across a "boundary". In the (proper) univariant case, divariant fields occur across the univariant, with the swapping of (just) one phase in the assemblage. However, the univariant case can be made to comply with all others by representing the univariant as an (infinitely) thin field involving the full univariant assemblage. Then the standard way of thinking about boundaries in pseudosections applies to univariants as well.

Points in pseudosections are where two modes are zero with respect to the lowest variance assemblage at the point. At a point there is one n + 1, two n, and one n - 1 variance fields. The two n - 1 to n variance field boundaries involve one each of the phases whose modes are zero at the point. In terms of calculation, these two boundaries terminate at the point, whereas the other two boundaries (n to n + 1 variance field boundaries) continue through the point. Considering a compatibility diagram, like the portion of AFM in (a) in Fig 3, and considering that the phase relations move with respect to the bulk composition (star) with changing PT, the variance relationships around points in PT pseudosections should be clear(er), as well as accounting for which lines will have metastable extensions.

Getting started in drawing a pseudosection is particularly straightforward if a univariant that is known to be stable (from the PT projection) is "seen" by the bulk composition (see below). Otherwise it is a matter of inspired guesswork, or Gibbs energy minimisation (via dogmin) can be used as a last resort.

Calculating along a line, 3 things can happen:

³it is possible that there will be an argument over whether this is a traducing of the variance idea, but I think not, in terms of number of equations and number of variables, *once* a bulk composition is specified...

- 1. the line is cut off by a *lower* variance field, with a new phase joining the equilibrium. If this line is a boundary between an n and an n+1 variant fields, then at the point where the line is cut off, an n-1, two n and an n+1 variant fields meet. Case (b) in Fig 3.
- 2. the line dies, with a mode going to zero. If this line is a boundary between an n and an n+1 variant fields, then at the point where the line is cut off, an n, two n+1 and an n+2 variant fields meet. Case (c) in the Fig 3.
- 3. THERMOCALC fails to calculate the line beyond a certain point, but no mode is going to zero. This signals a failure of the non-linear equation solver in THERMOCALC. The usual resolution is to vary the starting guesses in the datafile, using ones that correspond to the values along the univariant that THERMOCALC could calculate.

Calculating a point, 2 things can happen:

- 1. the point is calculated successfully.
- 2. THERMOCALC fails to calculate the point. This can arise for two reasons: 1. The qualitative assessment of the pseudosection geometry is flawed, and the point is not there to be found. This can easily happen locating where trivariants touch univariants, when a narrow field has been missed, for example. 2. A failure of the non-linear equation solver in THERMOCALC is signalled. As before, the usual resolution is to vary the starting guesses.

Calculating the part of a univariant that is "seen" is illustrated for our KFMASH example (using datafile TH DKA2):

```
chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : bi st g chl
fluid in excess (from script)
phases in excess: mu q (from script)
variance of required equilibria:
    0 = invariant
     1 = univariant
     2 = divariant
    n = n-variant
variance: 1
you may set zero modal proportions, from:chl bi st g mu q H2O
which to set : (nothing input)
equilibia now effectively univariant (eg a line in PT)
specification of PT window:
P range over which T of reactions to be calculated
P window: P low, high: 6 8.5
T window within which reactions expected to lie
T window: T low, high: (nothing input)
P window :6 <-> 9 kbar :P interval : 0.5
composition (from script)
 Al203 MgO FeO K20
 41.89 18.19 27.29 12.63
```

```
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
P(kbar)
             T(C)
                    x(chl)
                                       Q(chl)
                                                x(bi)
                                                         y(bi)
                                                                   Q(bi)
                             y(chl)
                                                                            x(st)
                                                                                      x(g)...
   6.00
            579.4
                    0.6017
                             0.5981
                                       0.4018
                                                0.6663
                                                         0.4169
                                                                  0.2107
                                                                           0.9155
                                                                                    0.9111...
       31chl + 23g + 74mu = 74bi + 10st + 125q + 103H20
            587.0
                    0.5602
                            0.5905
                                       0.4095
                                                0.6163
                                                         0.3747
                                                                  0.2582
                                                                           0.9005
                                                                                    0.8949..
   6.50
       32chl + 20g + 72mu = 72bi + 10st + 116q + 108H20
 mode
          chl
                   bi
                           st
       0.8709 0.1043
                               0.0248 0.4751
       0.7708 0.1916 0.0376
                                       0.4477
                             y(chl)
                                                         y(bi)
P(kbar)
             T(C)
                    x(chl)
                                       Q(chl)
                                                x(bi)
                                                                   Q(bi)
                                                                            x(st)
                                                                                      x(g)...
   7.00
                                                                  0.3002
                                                                           0.8855
                                                                                    0.8788...
            594.0
                    0.5238
                             0.5842
                                       0.4158
                                                0.5730
                                                         0.3392
       33chl + 19g + 70mu = 70bi + 10st + 110q + 110H20
 mode
          chl
                   bi
                                           mu
                                    g
       0.7660 0.1138
                               0.1202 0.4730
       0.3187 0.5079 0.1734
                                       0.3333
P(kbar)
             T(C)
                    x(chl)
                             y(chl)
                                      Q(chl)
                                                x(bi)
                                                         y(bi)
                                                                  Q(bi)
                                                                            x(st)
                                                                                      x(g)...
            600.4
   7.50
                    0.4909
                             0.5788
                                      0.4211
                                               0.5353
                                                         0.3101
                                                                  0.3357
                                                                           0.8705
                                                                                    0.8625...
       33chl + 17g + 69mu = 69bi + 10st + 105q + 112H20
 mode
                   bi
          chl
                               0.2008 0.4715
       0.6780 0.1212
               0.7258 0.2707 0.0035 0.2362
             T(C)
                                                                  Q(bi)
P(khar)
                    x(chl)
                             y(chl)
                                      Q(chl)
                                                x(bi)
                                                         y(bi)
                                                                           x(st)
                                                                                      x(g)...
   8.00
            606.5
                    0.4608
                             0.5742
                                      0.4258
                                               0.5022
                                                         0.2861
                                                                  0.3649
                                                                           0.8552
                                                                                    0.8458...
       33chl + 17g + 68mu = 68bi + 10st + 102q + 112H20
 mode
          chl
                   bi
                           st
                                    g
       0.6010 0.1274
                               0.2716 0.4703
               0.6711 0.2468 0.0821 0.2683
P(kbar)
             T(C)
                    x(chl)
                             y(chl)
                                      Q(chl)
                                                x(bi)
                                                         y(bi)
                                                                  Q(bi)
                                                                           x(st)
                                                                                      x(g)...
   8.50
            612.2
                                                         0.2663
                                                                  0.3881
                                                                           0.8396
                                                                                    0.8287...
                    0.4329
                             0.5700
                                      0.4299
                                               0.4728
       33chl + 16g + 67mu = 67bi + 10st + 100q + 112H20
 mode
          chl
                   bi
                                            mu
                                    g
       0.5310
               0.1329
                                0.3361
                                       0.4693
               0.6216 0.2242 0.1542
```

Looking at this output, no mode output is given for 6 kbar, but is for 6.5 kbar, signalling that the "seen" part of the univariant starts between these pressures. The two lines of mode information relate to the two sides of the reaction: across univariants is the *one* place in pseudosections that modes change discontinuously. Looking down pressure through the mode information, the modes of garnet and staurolite are both going to zero towards the end point of the univariant (so the point is bi chl (g st)). Looking at the high T side of the reaction, there is a change in the assemblage, signalling that the st + bi trivariant touches the univariant here (the point being st bi (g chl)). These points are easy to calculate, for example:

```
chl bi cd st ctd g mu ksp ky sill and q {\rm H2O}
which phases: bi st g chl
fluid in excess (from script)
phases in excess: mu q (from script)
variance of required equilibria :
    0 = invariant
    1 = univariant
    2 = divariant
    n = n-variant
variance: 1
you may set zero modal proportions, from:chl bi st g mu q H2O
which to set : g st
equilibia now effectively invariant (eg 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)
composition (from script)
A1203
      MgO
            FeO
41.89 18.19 27.29 12.63
<=========>>
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
                                              x(bi) y(bi)
            T(C)
                   x(chl)
P(kbar)
                            y(chl)
                                    Q(chl)
                                                              Q(bi)
                                                                       x(st)
                                                                                 x(g)...
                                             0.6271 0.3838 0.2477
   6.39
            585.3
                  0.5692
                           0.5921
                                    0.4078
                                                                       0.9039
                                                                               0.8986...
 mode
           chl
                    bi
                             st
                                              \mathtt{mu}
        0.3858 0.04366
                              0
                                          0.5705
```

Now, the g + chl + bi divariant on the low temperature side of the univariant goes into the chl + bi trivariant at the low pressure end of the "seen" part of the univariant, so there is the bi chl (g) line to calculate. So

```
chl bi cd st ctd g mu ksp ky sill and q H20
which phases : bi chl g
fluid in excess (from script)
phases in excess: mu q (from script)

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

```
you may set zero modal proportions, from:chl bi g mu q H20
which to set : g
equilibia now effectively univariant (eg a line in PT)
specification of PT window:
P range over which T of reactions to be calculated
P window: P low, high: 6 9
T window within which reactions expected to lie
T window: T low, high: (nothing input)
P window :6 <-> 9 kbar :P interval : 0.5
composition (from script)
 A1203
        MgO
             Fe0
 41.89 18.19 27.29 12.63
phases : chl, bi, g, (mu, q, fluid)
reactions : |XX|X|XXX|XX|-X
                                           x(bi) y(bi)
            T(C) x(chl)
                           y(chl)
                                    Q(chl)
                                                            Q(bi)
                                                                        x(g)...
                                                                      0.8981...
   6.00
            584.9
                   0.5687
                            0.6054
                                    0.3945
                                            0.6335
                                                     0.4219
                                                             0.2257
 mode
           chl
                    bi
                              g
        0.3769 0.06536
                              0
                                 0.5577
_____
             T(C)
                                             x(bi)
 P(kbar)
                   x(chl)
                            y(chl)
                                    Q(chl)
                                                      y(bi)
                                                              Q(bi)
                                                                        x(g)...
   6.50
            585.4
                   0.5692
                            0.5887
                                    0.4113
                                             0.6251
                                                     0.3727
                                                              0.2543
                                                                      0.8987...
 mode
           chl
                    hi
                                     mu
        0.3882 0.03771
                                 0.5741
                              0
                            y(chl)
 P(kbar)
             T(C)
                   x(chl)
                                    Q(chl)
                                             x(bi)
                                                      y(bi)
                                                              Q(bi)
                                                                        x(g)...
   7.00
            586.0
                   0.5686
                            0.5758
                                    0.4241
                                             0.6160
                                                     0.3272
                                                              0.2829
                                                                      0.8986...
 mode
           chl
                              g
        0.3977 0.01402
                                 0.5882
7777
```

Along this line to higher pressure, the mode of biotite is going to zero, signalling case (c) in Fig. 3. And so on. In this way a pseudosection is built up line-by-line and point-by-point.

Calculating compatibility diagrams

The constructional features of compatibility diagrams are illustrated in Fig. 4. The tie triangles (divariant equilibria) in the full system (within the triangle) as well as the divariant equilibria in the subsystems (edges of the triangle) specify much of the geometry, including the apices of the one-phase fields (quadrivariant equilibria). The edges of the one phase fields can be determined via the adjacent trivariant equilibria. In cases such as this, in which Fe–Mg is the dominant substitution, the edges are close to being straight; in other systems, such edges can be strongly curved. For example, running a divariant:

```
bi cd st ctd g mu ksp ky sill and q H2O
which phases: big chl
fluid in excess (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: 2
specification of PT window:
P range over which equilibria to be calculated
P window: P low, high: 8
T range over which equilibria to be calculated
T window: T low, high: 600
projection plane has 3 apices, leaving Al203 MgO FeO K20
to be represented by mu and the projection plane
projection plane (from script)
                   MgO
         A1203
                           FeΩ
                                   K20
         1.000
Α
                     0
                             0
                                      0
F
             0
                     0
                         1.000
                                      0
             0
                 1.000
                                      0
                             0
phases : chl, bi, g, (mu, q, fluid)
reactions : |XX|X|XXX|XX|-X
                                                           y(bi)
 P(kbar)
              T(C)
                              y(chl)
                                        Q(chl)
                                                                    Q(bi)
                     x(chl)
                                                  x(bi)
                                                                               x(g)...
   8.00
             600.0
                     0.4929
                              0.5682
                                        0.4317
                                                 0.5313
                                                          0.2726
                                                                   0.3606
                                                                             0.8639...
                    F
                            М
                                        phase
proj
            Α
                                   mıı
        0.189
                0.400
                        0.411
chl
                                        -0.167
bi
       -0.261
                0.643
                        0.618
                                0.500
                                       -0.500
                                        -0.250
        0.250
                0.648
                        0.102
g
```

The output gives the coordinates in the AFM triangle, the projection being from the *calculated* composition of muscovite, as well as quartz and H₂O.

Special cases and tricks-of-the-trade

1. In calculating univariants in PT projections, strongly curved ones and ones along which the phase change composition quickly can be awkward to calculate. One way to do this is to use isopleths (via the script "setiso"). If a phases composition, eg x(chl), changes progressively along the univariant, the univariant can be calculated as a series of effectively invariant points, each with a fixed value of x(chl). Running with TH DKA1A:

```
chl bi cd st ctd g mu ksp ky sill and q H2O
which phases : chl st g bi
fluid in excess (from script)
phases in excess: mu q (from script)
variance of required equilibria :
     0 = invariant
     1 = univariant
     2 = divariant
    n = n-variant
variance: 1
you may set compositional variables, from:
   x(chl) y(chl) Q(chl) x(bi) y(bi) Q(bi) x(st) x(g) x(mu) y(mu)
(maximum number to set = 1)
which variables to set : x(chl)
how to specify isopleth for x(chl):
 0: list of values
 1: start, finish, interval
isopleth: low, high, interval: 0.3 0.9 0.1
equilibia now effectively invariant (eg 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)
<=========>>
phases : chl, bi, st, g, (mu, q, fluid)
reactions : |XXX|X|X|XXX|XX|-X
P(kbar)
            T( C)
                   x(chl)
                             y(chl)
                                     Q(chl)
                                                        y(bi)
                                                                 Q(bi)
                                                                         x(st)...
                       0.3 0.5526
                                     0.4473
                                                       0.1981
                                                                0.4342
                                                                         0.7399...
            641.1
                                              0.3431
       32chl + 17g + 65mu = 65bi + 10st + 96q + 109H20
    9.13
            619.1
                       0.4
                            0.5654
                                     0.4346
                                              0.4394
                                                       0.2457
                                                                0.4100
                                                                        0.8193...
       33chl + 16g + 66mu = 66bi + 10st + 98q + 112H20
                                                                0.3262
                                                                         0.8748...
    7.36
            598.6
                       0.5
                            0.5803
                                     0.4197
                                              0.5456
                                                       0.3178
       33chl + 18g + 69mu = 69bi + 10st + 106q + 111H20
    6.02
            579.7
                       0.6 0.5978
                                     0.4021
                                              0.6642
                                                       0.4152
                                                                0.2126
                                                                         0.9149...
       31chl + 23g + 74mu = 74bi + 10st + 124q + 104H20
            562.5
                       0.7 0.6189
                                     0.3810
                                              0.7776
                                                       0.5100
                                                                0.1176
                                                                         0.9447.
       28chl + 31g + 79mu = 79bi + 10st + 147q + 90H20
           547.2
                       0.8
                                     0.3544
                                                       0.5806
                                                               0.05805
                                                                         0.9675...
                            0.6455
                                              0.8700
       24chl + 38g + 83mu = 83bi + 10st + 166q + 77H20
            533.7
                       0.9
                            0.6797
                                     0.3202
                                             0.9422
                                                       0.6300 0.02240
                                                                         0.9854...
       22chl + 43g + 86mu = 86bi + 10st + 180q + 67H20
```

2. Watch out for singularities, where phases change sides on reactions, along a reaction's length. Unless these are recognised, and they can be arbitrarily close to invariants, they can make a mess of the Schreinemakers analysis.

- 3. THERMOCALC does *not* tell which way around univariant reactions are. It makes a guess, but does not always get it right. (This is high up on my list of things to code. It is actually a non-trivial problem. [still not coded...])
- 4. Degenerate univariant equilibria, like law = $cz + ky + q + H_2O$ in NCFMASH, will be 'seen' by all lawsonite-bearing fields, regardless of their variance. Nevertheless, a divarant field that runs into this reaction will terminate in a *full* system univariant that can be calculated as such by THERMOCALC.

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