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Average *P-T* Documentation

Average *P-T* (or simply avPT) calculations are the standard THERMOCALC thermobarometry calculations (via calcmode 2). The essential reference regarding these calculations is (still)

> Powell, R, & Holland, TJB, 1994. Optimal geothermometry and geobarometry. *American Mineralogist*, 79, 120-133.

with the science behind the calculations, and the implementation in THERMOCALC not having changed since then. So this is a must-read regarding this type of calculation.

What has changed since then, with the development of the pseudosection approach of looking at the conditions of formation of rocks, is a move to use that approach for thermobarometry, rather than avPT. This is discussed in

> Powell, R, & Holland, TJB., 2008. On thermobarometry. *Journal of Metamorphic Geology*, 26, 155-180.

The logic behind avPT calculations is simple. Given a set of minerals (a mineral assemblage) that is interpreted to have once been in equilibrium, the end-members of the minerals (for which there is thermodynamic data in the internally consistent dataset) are used to write an independent set of reactions. For each reaction, an equilibrium relation can be written

$$0 = \Delta G^{o} + RT \ln K$$

in which ΔG^{o} is a function of just P and T, whereas K is a function of the composition of the minerals (primarily). If the end-members are in an n oxide system, and there are m end-members, then there are $m - n$ equilibrium relations. In avPT-type calculations, we know the activities (from the compositions of the minerals) which are used to calculate K, so each equilibrium relationship is a line in PT. The information for the several independent reactions is then combined in a least squares sense to calculate the conditions of formation

This can be done in several ways, depending on how much "information" is in the mineral assemblage. It may not be that calculating both P and T is possible (insufficient information). For example it commonly occurs that the temperature of formation of the rocks is already rather well known (by geological prejudice), in which case the focus of the calculations is on determining pressure (leading to the avP method). So:

- **average P** (or avP): The user nominates a T or a series of T and THERMOCALC calculates a series of avP values from the set of equilibrium relations.
- **average T** (or avT): The user nominates a P or a series of P and THERMOCALC calculates a series of avT values from the set of equilibrium relations.
- **average PT** Here both P and T are calculated from the set of equilibrium relations.

If additionally to PT there are other unknowns, for example the fluid composition (as in the following calculation), then avP, avT or avPT can be calculated for various values of the fluid composition.

To undertake calcmode=2 calculations, THERMOCALC reads a simple file of endmembers and their activities derived from mineral analyses (for example by electron probe microanalysis), usually produced by the separate software, Tim Holland's AX. Ax can be downloaded here, and instructions for using it can be viewed on the activity-composition documentation page.

When you have run AX, several output files are produced including a THERMOCALC-readable file. This file is your main input datafile. In this file you will need to add the names of any pure phases that also occur in your mineral assemblage (eg quartz, sillimanite, rutile, sphene etc), as well as H_2O and CO_2, as in the following example. an example of what this file looks like is given below. The datafiles used in the following example can be downloaded below.

Download datafiles for Mac

Download datafiles for PC

In the following example, for RP13 as used in the 1994 paper, a lower amphibolite facies calc-pelite that also contains calcite and quartz, AX was run with

```
SiO2 TiO2 Al2O3 Cr2O3 Fe2O3 FeO MnO MgO CaO Na2O K2O
mu rp13/mu
46.29 0.26 34.55 0.00 0.00 1.47 0.00 1.10 0.12 0.58 8.92
bi rp13/bi
37.61 1.40 18.19 0.00 0.00 16.62 0.00 12.47 0.09 0.11 7.63
fsp rp13/plag
59.93 0.00 25.28 0.00 0.00 0.00 0.00 0.00 6.17 8.07 0.19
ep rp13/ep
38.82 0.14 29.61 0.00 0.00 5.12 0.04 0.00 23.92 0.00 0.00
g rp13/gt
37.68 0.00 21.48 0.00 0.00 30.05 1.74 1.90 8.34 0.00 0.00
chl rp13/chl
25.39 0.00 22.75 0.00 0.00 21.97 0.02 17.56 0.04 0.00 0.00
*
```

THERMOCALC expects two input files, an axfile and a scriptfile, much as for mode 1 calculations. The axfile contains the activities of the end-members of the minerals for our calculations, and the scriptfile (which need contain only the first line in the example below) contains directions for the running of the calculation. One way of organising naming of files is to make the axfile (with the activities in) be

```
    tc-myrocknameax.txt
```

then the scriptfile be

```
    tc-myrockname.txt
```

THERMOCALC expects these files to be .txt files, and to start with tc-. (Note that in the prefs file, the scripts calcmode and scriptfile should not be set, such that you will be prompted for the calcmode and the name of the scriptfile).

This is the axfile used below, called tc-RP13ax.txt

```
%---------------------------------------------------
% axfile for RP13 - from AX at 8.0 kbar and 550.0 C
% (manually cleaned)

   mu        0.74
  cel       0.0117
 fcel       0.0026
   pa        0.217      % -> but other side of solvus

  phl        0.067
  ann        0.015
 east        0.066

   py      0.00152
   gr        0.016
```

```
  alm        0.24

 clin       0.056
 daph      0.0105
 ames       0.061

   cz        0.65

   an        0.48
   ab        0.70

cc q H2O CO2

*

% after this star, everything is just info for the record
% and is not read by THERMOCALC

=original=

   mu        0.74       0.037
  cel      0.0117      0.0040
 fcel      0.0026     0.00091
   pa       0.217      0.0185   % -> other side of solvus

  phl       0.067      0.0106
  ann       0.015     0.00395
 east       0.066      0.0105

   py     0.00152    0.000536
   gr       0.016     0.00415
  alm        0.24       0.018
% spss   0.000052  -> only Mn end-member

 clin       0.056      0.0089
 daph      0.0105     0.00293
 ames       0.061      0.0092

   cz        0.65       0.032
% ep         0.31  -> only Fe3+ end-member

   an        0.48      0.0193
   ab        0.70      0.0176
%---------------------------------------------------
```

It is definitely worth checking out what AX has produced before running it. It gives likely uncertainties on activities, on the basis of 1% relative uncertainty on the oxides in a probe analysis, but, as discussed in the 1994 paper these are very much minimum uncertainties and are overwritten by the default ones in THERMOCALC. So there is no particular use in including them, and they are omitted above. In this case, an obvious candidate for omission is paragonite (pa) as it is the dominant end-member on the other side of the white mica soluvs: its activity is not likely to be well-known in the mineral, muscovite (even though AX has had a go at suggesting what it might be). But initially, anyway we'll include it to see what happens.

The scriptfile, tc-RP13.txt, looks like

```
axfile RP13ax       % where the activities are

setrockname RP13

fluidpresent

setPwindow 3 12     % just specifying the P window for the calculations
setlinear 1         % specifying how linear the equilibria need to be to be used

progress no
```

```
*
```

with the critical line being the first one, telling THERMOCALC where the activities for the calculation are to be found.

We will run this with avP as we think we know more or less the temperature it is likely to have formed at (540°C or so), from the geology of the area and our petrological prejudice for moderate pressure lower amphibolite facies rocks. the following is from the logfile, putting in a range of temperature around our estimate, and a value of x(CO_2) = 0.25 (just as a first guess)

```
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  : 2
[display/print with fixed width font (eg Monaco)]

THERMOCALC 3.35  running at 20.36 on Sun 11 Apr,2010
suffix to name for script info datafile : RP13
the main output is in the file, "tc-RP13-o.txt"
other (eg drawpd) output is in the file, "tc-RP13-dr.txt"

calcs use: tc-ds55.txt produced at 19:29:59 on 22 Nov 2003 (with sigma fit =  1.067)

reading a-x datafile, "tc-RP13ax.txt"...
mu  cel  fcel  pa  phl  ann  east  py  gr  alm  clin  daph  ames  cz  an  ab
cc  q  H2O  CO2

mu  cel  fcel  pa  phl  ann  east  py  gr  alm  clin
daph  ames  cz  an  ab  cc  q  H2O  CO2
which end-members : (nothing input)
type of rock calculation:
       1 : average P
       2 : average T
       3 : average PT
code : 1

  RP13       mu      cel     fcel       pa      phl      ann     east       py       gr      alm
     a    0.740   0.0117  0.00260    0.217   0.0670   0.0150   0.0660  0.00152   0.0160    0.240
 sd(a)   0.0740   0.0100   0.0100   0.0399   0.0221  0.00766   0.0219  0.00107  0.00806   0.0360

           clin     daph     ames       cz       an       ab       cc        q      H2O      CO2
     a   0.0560   0.0105   0.0610    0.650    0.480    0.700     1.00     1.00
 sd(a)   0.0196  0.00576   0.0208   0.0325   0.0389   0.0350        0        0

these data ok ? yes

specification of PT window:
P window : 3.0 <=> 12.0 kbar (from script)
T range over which average P to be calculated
T window: T low,high :  480 600
T window : 480 <-> 600°C :T interval : 20
fluid is just H2O-CO2
fixed x(CO2) : 0.25
reactions :
|:|0|0|:0|X00X0-X|X|0:0::|---|00X00::X0000000-00000000000000-000:X|0
0000|X0:000|0|-----------|------------------------------------------------------
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
------------------------------------------------------------------|0X-----------
-----------------------------------------------|X------|----:-------::-::-::----
-0----------0-0--000----0----0-0-:---00---00--0-00-0-0--00-:00000:---000000-:000
0:--00000------:---------:X
```

```
an independent set of reactions has been calculated

Activities and their uncertainties for RP13

                mu      cel     fcel       pa      phl      ann     east
a            0.740   0.0117  0.00260    0.217   0.0670   0.0150   0.0660
sd(a)/a    0.10000  0.85470  3.84615  0.18393  0.32959  0.51082  0.33131

                py       gr      alm     clin     daph     ames       cz
a          0.00152   0.0160    0.240   0.0560   0.0105   0.0610    0.650
sd(a)/a    0.70494  0.50357  0.15000  0.34963  0.54900  0.34022  0.05000

                an       ab       cc        q      H2O      CO2
a            0.480    0.700     1.00     1.00    0.750    0.250
sd(a)/a    0.08112  0.05000        0        0

Independent set of reactions
1)  4gr + clin + ames + 20an = 3py + 16cz
2)  py + 2gr + 3ames + 6q = 3clin + 6an
3)  2gr + 3clin + 18an = 5py + 12cz + 6H2O
4)  5alm + 24cz + 3q = 5gr + 3daph + 33an
5)  mu + 2phl + 6q = 3cel + py
6)  2east + 6q = mu + cel + py
7)  2phl + ames + 6q = 2cel + py + clin
8)  mu + 2ann + 6q = 3fcel + alm
9)  ann + 3an = mu + gr + alm
10)  5alm + 30cz + 3ab = 3pa + 8gr + 3daph + 36an
11)  5mu + 24fcel + 7py + 12cc = 21cel + 8ann + 12an + 12CO2

Calculations for the independent set of reactions
 at T = 540°C  (for x(CO2) = 0.25 and x(H2O) = 0.75)
        P(T)   sd(P)       a   sd(a)         b        c     ln_K sd(ln_K)
1        8.1    0.60 -250.27    4.98   0.62150  -40.051   10.540    3.470
2       10.6    1.14    7.67    1.89  -0.24606   11.765   10.099    1.972
3        8.4    0.77  187.43    3.99   0.21256  -36.802   -7.486    4.127
4        8.4    0.46  598.77    9.15  -1.07789   65.801  -41.092    4.269
5        5.8    4.31   81.64    1.14   0.04770   -4.303  -14.126    2.742
6        4.5    2.37   36.58    1.11   0.02381   -3.730   -5.802    1.295
7        4.1    3.73   62.10    1.04   0.02530   -3.672  -10.065    2.023
8        4.6   16.61   63.31    2.19   0.03626   -4.717  -10.583   11.585
9        9.5    0.73  -37.16    1.15   0.12706   -7.373    0.538    0.779
10       8.9    0.57  663.85   10.70  -1.09397   68.258  -56.628    5.533
11       5.7   12.58  228.87   12.62  -1.08229   50.661   53.966   94.261

corresponding average P

         avP     sd   fit
lsq     7.48   0.67  2.76

diagnostics on this average P

for 95% confidence, fit (= sd(fit) = sqrt(MSWD)) < 1.35 (but larger may be OK)

column:
1-3: result of doubling the uncertainty on ln a.
4: e* = ln a residuals normalised to sd(ln a) : |e*| >2.5 suspect?
5: hat = diagonal elements of the hat matrix : hat >0.55 influential.
6-7: observed and calculated activities of endmembers.
8-9: regression-through-origin x,y values

              P     sd    fit     e*   hat    a(obs)   a(calc)      x      y
      mu   7.40   0.68   2.73   -0.8  0.03     0.740     0.681   0.71   6.17
     cel   7.48   0.67   2.75    0.8  0.00    0.0117    0.0241  -0.11  -1.68
    fcel   7.48   0.67   2.75    0.5  0.00   0.00260    0.0168  -0.03  -0.74
      pa   8.24   0.52   1.91    6.1  0.23     0.217     0.662   1.98   8.74
     phl   7.35   0.68   2.69    1.9  0.08    0.0670     0.124  -1.15 -10.48
```

```
      ann   7.32   0.65   2.60    3.0  0.06    0.0150    0.0710  -0.99 -10.43
     east   7.52   0.66   2.72   -1.4  0.02    0.0660    0.0408  -0.52  -2.43
       py   7.48   0.67   2.76    0.1  0.00   0.00152   0.00166   0.29   2.04
       gr   7.47   0.67   2.76    0.4  0.02    0.0160    0.0197  -0.60  -4.90
      alm   7.43   0.66   2.71   -1.2  0.01     0.240     0.201   0.40   4.14
     clin   7.50   0.65   2.69    1.8  0.00    0.0560     0.104   0.16  -0.55
     daph   7.48   0.67   2.75    0.6  0.00    0.0105    0.0145  -0.24  -2.35
     ames   7.32   0.64   2.58   -3.0  0.04    0.0610    0.0222   0.87   9.46
       cz   7.46   0.67   2.74   -0.8  0.00     0.650     0.626   0.26   2.73
       an   7.15   0.80   2.69    1.7  0.38     0.480     0.549  -2.53 -20.63
       ab   7.62   0.65   2.62   -1.6  0.02     0.700     0.645  -0.54  -2.38
       cc   7.48   0.67   2.76      0     0      1.00      1.00      0      0
        q   7.48   0.67   2.76      0     0      1.00      1.00      0      0
      H2O   7.48   0.67   2.76      0     0      1.00      1.00      0      0
      CO2   7.48   0.67   2.76      0     0      1.00      1.00      0      0


Average pressures for RP13 (for x(CO2) = 0.25 and x(H2O) = 0.75)

T°C       480   500   520   540   560   580   600
av P      4.9   5.8   6.6   7.5   8.3   9.2  10.0
sd       0.75  0.75  0.70  0.67  0.67  0.72  0.80
sigfit    3.8   3.3   3.0   2.8   2.7   2.8   3.0
```

For the meaning of the output, and particularly the diagnostics, read the 1994 paper. Having already suggested that pa may not be useful, note that e* for pa (a measure of how consistent its activity is with the rest of the data) is large, flagging that its inclusion might be problematic. Note in particular that the overall sigfit (a measure of whether the data are playing well with each other) is rather large (2.8, rather than <1.35, say), it is worthwhile rerunning omitting pa:

```
more calculations with this rock ? yes

**************************************

type of rock calculation:
       1 : average P
       2 : average T
       3 : average PT
code : 1

  RP13        mu       cel      fcel        pa       phl       ann      east        py        gr       alm
     a     0.740    0.0117   0.00260     0.217    0.0670    0.0150    0.0660   0.00152    0.0160     0.240
 sd(a)    0.0740    0.0100    0.0100    0.0399    0.0221   0.00766    0.0219   0.00107   0.00806    0.0360

            clin      daph      ames        cz        an        ab        cc         q       H2O       CO2
     a    0.0560    0.0105    0.0610     0.650     0.480     0.700      1.00      1.00
 sd(a)    0.0196   0.00576    0.0208    0.0325    0.0389    0.0350         0         0

these data ok ? no
names of end-members to be excluded : pa
these are the only changes you want to make ? yes

specification of PT window:
P window : 3.0 <=> 12.0 kbar (from script)
T range over which average P to be calculated
T window: T low,high :  480 600
T window : 480 <-> 600°C :T interval : 20
fluid is just H2O-CO2
fixed x(CO2) : 0.25

... (output omitted)

diagnostics on this average P

for 95% confidence, fit (= sd(fit) = sqrt(MSWD)) < 1.37 (but larger may be OK)
```

```
column:
1-3: result of doubling the uncertainty on ln a.
4: e* = ln a residuals normalised to sd(ln a) : |e*| >2.5 suspect?
5: hat = diagonal elements of the hat matrix : hat >0.56 influential.
6-7: observed and calculated activities of endmembers.
8-9: regression-through-origin x,y values

            P     sd    fit     e*   hat    a(obs)   a(calc)      x      y
     mu  8.71   0.38   1.27    0.3  0.05     0.740     0.765   0.79   6.52
    cel  8.65   0.36   1.27    0.5  0.00    0.0117    0.0183  -0.16  -1.88
   fcel  8.65   0.36   1.28    0.4  0.00   0.00260    0.0121  -0.05  -0.79
    phl  8.67   0.39   1.28   -0.1  0.14    0.0670    0.0652  -1.31 -11.17
    ann  8.54   0.36   1.20    1.4  0.10    0.0150    0.0239  -1.10 -10.92
   east  8.74   0.32   1.10   -2.1  0.02    0.0660    0.0223  -0.53  -2.50
     py  8.67   0.36   1.27    0.6  0.01   0.00152   0.00183   0.31   2.13
     gr  8.67   0.37   1.28   -0.3  0.03    0.0160    0.0129  -0.60  -4.91
    alm  8.62   0.36   1.26   -0.5  0.02     0.240     0.185   0.44   4.33
   clin  8.68   0.31   1.08    1.9  0.00    0.0560    0.0749   0.16  -0.57
   daph  8.65   0.37   1.28    0.2  0.01    0.0105    0.0113  -0.26  -2.44
   ames  8.53   0.35   1.18   -1.4  0.08    0.0610    0.0282   1.00  10.04
     cz  8.70   0.37   1.26    0.5  0.02     0.650     0.764   0.48   3.69
     an  8.78   0.47   1.27   -0.5  0.44     0.480     0.469  -2.33 -19.74
     cc  8.66   0.37   1.28      0     0      1.00      1.00      0      0
      q  8.66   0.37   1.28      0     0      1.00      1.00      0      0
    H2O  8.66   0.37   1.28      0     0      1.00      1.00      0      0
    CO2  8.66   0.37   1.28      0     0      1.00      1.00      0      0


Average pressures for RP13 (for x(CO2) = 0.25 and x(H2O) = 0.75)

T°C       480   500   520   540   560   580   600
av P      6.1   7.1   7.9   8.7   9.4  10.2  11.0
sd       0.63  0.52  0.41  0.37  0.43  0.57  0.75
sigfit    2.7   2.0   1.5   1.3   1.5   1.9   2.4
```

Now definitely sigfit is in a good range, so we should not be looking at the diagnostics to omit anything further. If we are happy with our guess for tempearture (540°C) and fluid composition (x(CO_2) = 0.25), then we have a pressure estimate of 8.7 ± 0.74 kbar (noting that we use double the sd for the quoted ±)

We can easily see how the avP varies with specified fluid composition and temperature by rerunning

```
T°C       480   500   520   540   560   580   600
av P      6.4   7.2   8.0   8.8   9.6  10.4  11.2   x(CO2) = 0.15
sd       0.67  0.55  0.47  0.48  0.58  0.74  0.93
sigfit    2.6   2.0   1.7   1.7   2.0   2.4   3.0

T°C       480   500   520   540   560   580   600
av P      6.1   7.1   7.9   8.7   9.4  10.2  11.0   x(CO2) = 0.25
sd       0.63  0.52  0.41  0.37  0.43  0.57  0.75
sigfit    2.7   2.0   1.5   1.3   1.5   1.9   2.4

T°C       480   500   520   540   560   580   600
av P      6.2   6.9   7.8   8.6   9.4  10.2  11.0   x(CO2) = 0.35
sd       0.67  0.52  0.39  0.33  0.37  0.50  0.67
sigfit    2.6   2.0   1.4   1.2   1.3   1.7   2.2

T°C       480   500   520   540   560   580   600
av P      6.2   6.9   7.7   8.5   9.3  10.1  10.9   x(CO2) = 0.45
sd       0.67  0.52  0.40  0.33  0.36  0.48  0.64
sigfit    2.6   1.9   1.5   1.2   1.2   1.6   2.1

T°C       480   500   520   540   560   580   600
```

```
av P       6.2    6.9    7.7    8.5    9.3   10.2   11.0   x(CO2) = 0.55
sd        0.67   0.53   0.42   0.37   0.40   0.51   0.66
sigfit     2.6    2.0    1.5    1.3    1.4    1.7    2.2

T°C        480    500    520    540    560    580    600
av P       6.2    7.0    7.8    8.5    9.4   10.3   11.1   x(CO2) = 0.55
sd        0.66   0.55   0.47   0.46   0.50   0.60   0.74
sigfit     2.6    2.1    1.7    1.7    1.7    2.0    2.4
```

We can see from this that the pressure at a particular estimated temperature is rather insenstive to fluid composition for this particular mineral assemblage (but may well not be for other ones)

In fact we can easily leave out calcite and the fluid end-members, and get a result which makes no assumption about fluid composition (or even presence), and this gives

```
Average pressures for RP13

T°C        480    500    520    540    560    580    600
av P       7.5    7.9    8.3    8.7    9.0    9.4    9.8
sd        0.40   0.41   0.42   0.43   0.45   0.47   0.50
sigfit     1.2    1.2    1.2    1.2    1.3    1.3    1.3
```

Given a conceivable uncertainty on estimated temperature, and the lack of dependence on fluid composition, it would be reasonable to suggest that the mineral assemblage reflects a pressure of 8.5 ± 1 kbar

As a postscript to this brief introduction to avPT calculations, it should be noted that a new way of inputting activities for avPT calculations is outlined in the 2008 "On thermobarometry" paper, involving using mode 1 axfiles. However, in general, until more detailed axfile descriptions of phases are available, continuing to use AX is recommended. Watch this space.

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