Computer Programs for P-T Calculations and Construction of Phase Diagrams: Use of TWQ, WEBINVEQ and THERMOCALC

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Abstract

Reconstruction of the P -T-t path followed by crustal rocks during orogeny has assumed greater sign ficance.This paper reviews and discuss with examples use and applications of computer programs TWQ (Berman, 1991). WEBINVEQ (Gordon 1998) and THERMOCALC (Powell and Holland 1988; Holland and Powell 1998) for P-T calculations and construction of phase diagrams. TWQ is an interactive prog am for calculation of mineral fluid equilibria Its primary application is geothermobarometry Included in the DOS package are programs for convert ng microprobe analyses to mineral formulae used by TWQ, calculating P- T curves, plotting and making DXF files that can be imported into various graphics packages such as COREL DRAW, WEBINVEQ is in interactive scient fic software for thermobarometnc calculat ons on the World Wide Web WEBINVEQ thermobarometry uses an approach that provides some advantages in analyzing and solving the inverse chemical equilibrium problem in metamorphic petrology. It is a generalization of classical thermobarometry hence of interest to geologists who are studying metamorphic rocks. The mathematical problem is the determination of the weighted non linear least squares solution to a set of polynomial functions in the unknown pressure (P) temperature (T) and a problem dependent set of chemical potentials ( )

THERMOCALC is a thermodynamic calculation soltware for solving mineral equilibna problems. It has two main components the application itself and the internally consistent thermodynamic dataset it uses .The mineral equilibria problems that can be addressed with THERMOCALC include *inverse modelling* (geothermometry/barometry using average FT) and *forward modelling* (calculating phase diagrams for model systems) Quantitative phase diagrams involving solid solutions can be calculated including P- T projections compatibility diagrams P- T, T- X and P- X pseudosect ons for specific bulk compositions .In the last decade, this approach has been successfully applied to solving the phase relations, P- T conditions and evolution histories of rocks in pelitic and the mafic systems. Some test runs are generated for demonstrating use of these computer programs along with P-T estimates done on the Dudatoli- Almora crystallines Garhwal- Kumaun Lesser Himalaya in order to place quantitative constraints on the conditions attained during the regional metamorphism.

Introduction

Reconstruction of the P-T-t path followed by crustal rocks during orogeny has assumed greater significance. This paper reviews and discusses with examples, use and applications of computer programs TWQ (Berman, 1991; http://www.gis.nrcan.gc.ca/twq.html) WEBINVEQ (Gordon 1998) and THERMOCALC (Powell and Holland 1988; Holland and Powell, 1998) for P-T calculations and construction of phase diagrams. Some test runs are generated for demonstrating use of these computer programs along with P-T estimates done on the Dudatoli-Almora crystallines, Garhwal-Kumaun Lesser Himalaya in order to place quantitative constraints on the conditions attained during the regional metamorphism.

TWQ

TWQ is an interactive program for calculation of mineral-fluid equilibria. It has been developed and maintained by R.G.Berman and T.H.Brown of the Geological Survey of Canada. Its primary application is geothermobarometry. Included in the DOS package, are programs for converting microprobe analyses to mineral formulae used by TWQ calculating P-T curves, plotting and making DXF files that can be imported into various graphics packages such as COREL DRAW. Program versions for IBM compatible machines can be downloaded from the following web site: http://www.gis.nrcan.gc ca/twq.html

TWQ 1.02 (version 1.02 ZIP/DOC) - June 1992

Version 1.02 TWQ program, documentation on running TWQ and other programs, thermodynamic data of Berman (1988) with amphibole thermobarometry capabilities from Mader et al. (1994).

TWQ 2.01 (version 2.01 ZIP/DOC) - October, 1996

Version 2.01 TWQ program, thermodynamic data of Berman (1988) updated with internally consistent solid solution and end-member data for:

(a) gt, ol,opx,cd, ilmenite from Berman & Aranovich (1996)

(b) clinopyroxene (Berman et al. 1995)

(c) biotite, spinel

Other files that can be downloaded from this site include

PKUNZIP.EXE: program to unzip files

GTCPX.ZIP: program for calculating gt-cpx temperatures

B88.MIN : TWQ format thermodynamic data of Berman (1988)

One should read the documentation associated with each program version before trying to use this software. Full documentation (TWQ.DOC) for running TWQ and auxiliary programs is contained in the TWQ102 package (Zip file). Documentation for new TWQ features, auxiliary programs, and thermodynamic data are contained in the TWQ201 and TWQ202 Zip files. TWQ version 1.02 (TWQ 102) is the earliest release and contains the complete documentation for operation of the TWQ program as well as auxiliary programs. This version also includes capabilities for doing amphibole thermobarometry.

Figure. 1. shows the phase diagram of the andalusite, kyanite and sillimanite, drawn utilizing TWO 2.02.

WEBINVEQ with the TWQ1.02 database

Gordon (1998) provided an interactive scientific software for thermobarometric calculations on the World Wide Web. Since specialized scientific software is volatile and often has a small number of users with a wide variety of computer platforms. The problems of distributing, updating and maintaining such packages can be replaced by using the World Wide Web to distribute graphical interface processing to individual user's web browsers and performing the numerical computations on a single server. This application uses perl as the CGI scripting language and MATLAB (The MathWorks (1995) as the computational language. MATLAB is a high-level programming language that incorporates many advanced numerical algorithms and flexible graphical output. It is widely used in the scientific and engineering communities and is available for personal computers running on Microsoft Windows, Macintosh and Unix operating systems (Marcotte, 1991).

WEBINVEQ thermobarometry uses an approach that provides some advantages in analyzing and solving the inverse chemical equilibrium problem in metamorphic petrology (Gordon, 1992; Gordon et al. 1994). It is a generalization of classical thermobarometry, hence useful for studying metamorphic rocks. The mathematical problem is the determination of the weighted non-linear least-squares solution to a set of polynomial functions in the unknown pressure (P), temperature (T) and a problem dependent set of chemical potentials ( ).

Initially, compositions of the theoretical end-members under investigation are selected and assembled into a matrix. The difference between the number of columns and rank of this matrix determines whether or not the problem is underdetermined, exactly determined or overdetermined. If the problem is not underdetermined, a solution for pressure and temperature can be obtained. In this situation, the coefficients in the polynomials are retrieved from the database and the resulting set of equations solved either exactly or in a least-square sense.

The solution includes estimates of the values of the unknowns and an approximation to the covariance matrix of errors in the solution, which can be displayed as an ellipse.

The computer implementation can be subdivided into

(i) user input;

(ii) database retrieval;

(iii) interfaces to and from computational procedures and

(iv) computational procedures.

WEB site address of WEBINVEQ is:
http://www.ichor.geo.ucalgary.ca/~tmg/webinveq/rgb95.html

Using WEBINVEQ to obtain a pressure-temperature estimate is a two-step process

1. Initial Request Form - This form contains a list of mineral end-members for which standard state thermodynamic data are available in the TWQ1.02 data base (Berman, 1988). Submitting this form with a selection of mineral end-members will return a web page containing:
   - An analysis of the feasibility of solving the inverse chemical equilibrium problem with the chosen end members; and (if the problem can be solved)
   - A second form that takes as input the activities and uncertainties you wish to assign to each end-member
2. Submitting the second form will return the pressure-temperature error analysis as described in Gordon (1992), Gordon et al. (1994) and Ghent and Gordon (2000).

Text Example

- Select Sillimanite, andalusite and Kyanite on the form
- Click on the Submit button at the bottom of the form
- Submit the second form with the default activities, uncertainities and plot options
- WEBINVEQ will return a page giving the computed temperature and pressure of the triple point, a table showing the problem is exactly determined , and a plot showing the computed pressure and temperature and error ellipses.

Thermocalc

THERMOCALC (by Powell and Holland) is a thermodynamic calculation software for tackling mineral equilibria problems. It has two main components: the application itself, and the internally-consistent thermodynamic dataset it uses. The mineral equilibria problems that can be addressed with THERMOCALC include *inverse modelling* (geothermometry/barometry using average PT), and *forward modelling* (calculating phase diagrams for model systems). THERMOCALC and associated program AX and DRAWPD are written in Pascal using Metrowerks Codewarrior on the Mac platform, and Delphi on the PC platform. The PC development is done on the Mac using the emulsion software, RealPC, running Windows 95.

The first thermodynamic calculation program with the name THERMOCALC (in FORTRAN language) was written by Roger Powell in 1971. It went through various modifications over the years from mainframes to Hewlett-Packard programmable calculators.

The latest version of THERMOCALC (version 3.1, June 2001) can be downloaded from the Roger Powell's THERMOCALC homepage: http://www.earthsci.unimelb.edu.au/tpg/thermocalc/ or from web site http://www.esccam.ac.uk/astaff/holland/thermocalc.html

THERMOCALC, being backwards-compatible, works with the various generations of dataset, so it is usually appropriate to use the current version of THERMOCALC, as available from the above mentioned web sites. Which version of the thermodynamic dataset one uses is more important? There are two mam versions of THERMOCALC currently available:

- "Tutorial" involves the 20apr96 dataset, and the documentation related to "tutorial" (see web site of Roger Powell, University of Melbourne http://www.earthsci.unimelb.edu.au/tpg/thermocalc/)uses that dataset. The tutorial dataset can be used, for example, for teaching or learning purposes, as it uses the simpler solid-solution models of Holland and Powell (1990).
- The HP98 dataset: For research work, the HP98 dataset (Holland and Powell, 1998) incorporating the most recent calorimetric and experimental data should be used. Some preliminary documentation on the dataset (and activity-composition relations) and the program THERMOCALC is available from http://www.esc.cam.ac.uk/astaff/holland/thermocalc.html

The new dataset makes more use of non-ideal solutions, the data files are more complex, especially for new users of THERMOCALC.

The THERMOCALC version 3.1, June 2001 is available for IBM PC/ compatibles: as a 32-bit executable binary to run under DOS or under windows.

How to run THERMOCALC

. Before running THERMOCALC, you must have a datafile for your rock or model system (depending on whether one is doing inverse or forward modelling)

. THERMOCALC is a standard (old-fashioned) "console" application, so when we run it, it operates by Question & Answer. Proceed by answering questions that it asks you (statements ending in "?": to answer yes, just hit return, or type 1 or y or yes, then return; to answer 'no', type O or n or no, then return) or giving information, then hit return, or, in some cases, just hitting return uses a default).

. Besides the information on the screen, THERMOCALC puts essential output into a file (a TH 0 file), a complete log file (the TH LOG file), and also specially formatted output, for example, for use by the software DRAWPD, into a file (the TH DR file).

The steps in phase diagram calculations

- Datafile creation (a-x relationships, bulk composition etc) for THERMOCALC
- Calculation of component parts of phase diagram (often line-by-line) by THERMOCALC
- Manual assembly of THERMOCALC output for input to DRAWPD
- Generation of postscript drawing by DRAWPD
- Labelling the phase diagram with Adobe Illustrator (or other postscript graphics program)

Some THERMOCALC related references are Guiraud et al. (1990), Holland and Powell (1985,1990,1998,2001), Powell and Holland (1985, 1988, 1993, 1994, 2001), Powell and Smith (1973), Powell et al. (1998), Wei et al. (2003) and White and Powell (2002).

Geothermobarometry of the Dudatoli-Almora Crystallines

The Garhwal and Kumaun regions of the Himalaya in Uttaranchal State of India are critical areas for studying the typical characteristics of the Himalayan fold-and-thrust belt, in contrast to the areas in close proximity of the northeast and northwest Himalayan syntaxes, where complications arise due to strike-slip faulting. In this region, the Lesser Himalaya is characterized by the occurrence of many crystalline bodies of varying dimensions, of which synformally disposed Dudatoli-Almora Crystalline Zone (ACZ) is the largest. Dudatoli-Almora Crystallines (also called Almora Klippen) constitutes one of the most important

tectonic units in the Garhwal-Kumaun Lesser Himalaya and it is the remnant of a large thrust sheet nappe that moved southward from the Higher Himalayan Crystalline Zone, to rest over the Lesser Himalayan Volcano-Sedimentary belt. The Almora klippen consists of amphibolite grade metapelites, quartzites, augen gneisses and granites belonging to the Precambrian Almora Group. At places, the greenschist grade metapelites of the Precambrian Ramgarh Group (Chails) occur underneath the Almora Group, forming a series of lower klippen.

The North Almora Thrust (NAT) marks the northern boundary of the Almora klippen, its southern margin is bound by the South Almora Thrust (SAT). The metamorphic sequence of the Almora Klippen exhibits regional metarnorphism of Barrovian type, which increases progressively upward in the sequence from peripheral part to the central part of the synform. In Champawat and Almora areas the metamorphism is largely restricted to the chlorite, biotite and garnet zones; however, in the Dudatoli-Bungidhar regions, the metamorphic grade reaches upto staurolite-kyanite and biotite-sillimanite zones (Jowhar and Rawat, 2004).

The EPMA data on garnet, biotite, muscovite and plagioclase was obtained on twenty samples collected from Chamoli, Pauri and Almora districts of Garhwal and Kumaun Himalaya, by utilizing JEOL-8600 M electron microprobe. In the garnet rim, (X_{Mg}/X_{Fe}) varies from 0.053 to 0.297, $X_{Almandine}$ vanes from 0.488 to 0.780 and (Ca+Mn)/(Ca+Mn+Fe+Mg) varies from 0.065 to 0.423. In the garnet core, (X_{Mg}/X_{Fe}) varies from 0.030 to 0.279, $X_{Almandine}$ varies from 0.487 to 0.753 and (Ca+Mn)/(Ca+Mn+Fe+Mg) varies from 0.118 to 0.461. Ti in garnets is significantly low, in the rim it varies from 0.004 to 0.012 and in cores 0.008 to 0.115. In the rim of biotite grains, (X_{Mg}/X_{Fe}) varies from 0 513 to 2.245, (Al^{VI}+Ti)/ (Al^{VI}+Ti+Fe+Mg) varies from 0.142 to 0.204 and $X_{Phlogopite}$ from 0.270 to 0.579. In the core of biotites, (X_{Mg}/X_{Fe}) varies from 0.547 to 2.198, (Al^{VI}+Ti)/ (AI^{VI}+Ti+Fe+Mg) varies from 0.125 to 0.216 and $X_{Phlogopite}$ from 0.277 to 0.581. In all the samples from Dudatoli-Almora crystallines (Ca+Mn)/(Ca+Mn+Fe+Mg) in garnets exceeds value of 0.2 or (AI^{VI}+Ti)/(AI^{VI}+Ti+Fe+Mg) in biotite exceeds value of 0.15. P-T estimates have been done on the Dudatoli-Almora Crystallines in order to place quantitative constraints on the conditions attained during the regional metamorphism. P-T calculations were carried out using computer programs TWQ (Berman, 1991), WEBINVEQ (Gordon, 1998), THERMOCALC (Powell and Holland 1988; Holland and Powell, 1998) and BGT (Jowhar, 1999). It is interpreted that in Dudatoli-Almora Crystallines T varies from 500 to 650 °C and P from 6 to 8 kbar. Table 1 and 2, and Figure 2 show result obtained by TWQ1.02 on sample no. R9-124 garnet mica schist (sample location: right bank of Eastern Nyar, Marora village) from Almora crystallines. Table 3 and figure 3 gives WEBINVEQ results for sample no. R9-124 using the TWQ 1.02 database.

Table 1 : Input Data File for Sample No. R9-124

```
GARN  [-Gr-][-Py-][-Alm][-Sp-]
GARN  .030  .193  .649  .129
MICA  [-xK-][-xNa][xAl-][-xOH]
MICA  .650  .349  .874  1.00
BIOT  [xMg-][xFe-][-xT1][-xAl][-xK-][-xOH]
BIOT  .559  .249  .023  .135  .783  1.0
PLAG  [-An-][-Ab-][-Or-]
PLAG  .080  .916  .004
FIXED ACTIVITY
SILLIMANITE=1.0
ENDFIX
```

Table 2 : Results for Sample No. R9-124 using TWQ1.02

```
plot dat
Intersections discarded with slope differences less than 20 degrees
Number of independent reactions =  3

#   Equilibrium

  1: 2 Si + aQz + Gr = 3 An
  2. Alm + Ms = 2 Si + aQz + Ann
  3. Phi + Alm = Ann + Py
  4: Ms + Gr + Alm = Ann + 3 An
  5: Py + Ms = Phl + aQz + 2 Si
  6: Py + Ms + Gr = 3 An + Phl

 Tot Ints # Used   Yavg     Ydev      Xavg      Xdev
     6       6   7654.69   167.27    498.60     7.29

 # INTERSECTIONS OUTSIDE DIAGRAM LIMITS =  3
 # INTERSECTIONS DISCARDED DUE TO PARALLELISM =  6

 Reaction  Intersection use:    dS       dV      dSdV/RlnK"
    1      1                  -111.1    -5.45     4.0269
    2      1                   -21.8    -2.12     0.8683
    3      2                   -13.7    -0.31     0.0403
    4      1                  -132.9    -7.57     4.9404
    5      5                    -8.2    -1.81     0.2329
    6      2                  -119.2    -7.26     4.0503
```

Refining average by discarding intersections outside of 1.5 sigma

Tot Ints	# Used	Yavg	Ydev	Xavg	Xdcv
6	4	7612. 50	108 .26	496.07	5.89

Results based on independent set of reactions

Reaction	Intersection use	dS	dV	dSdV/RlnK"
1	1	-111.1	-5.45	4.0269
2	1	-21.8	-2.12	0.8683
3	0	-13 .7	-0.31	0. 0403
4	1	-132 .9	-7..57	4. 9404
5	4	-8.2	-1.81	0.2329
6	1	-119.2	-7.26	4.0503

Equilibria more than 1.5 Sigma outside average P- T

3: Phl + Alm = Ann + Py

Ann has level 3 reliability

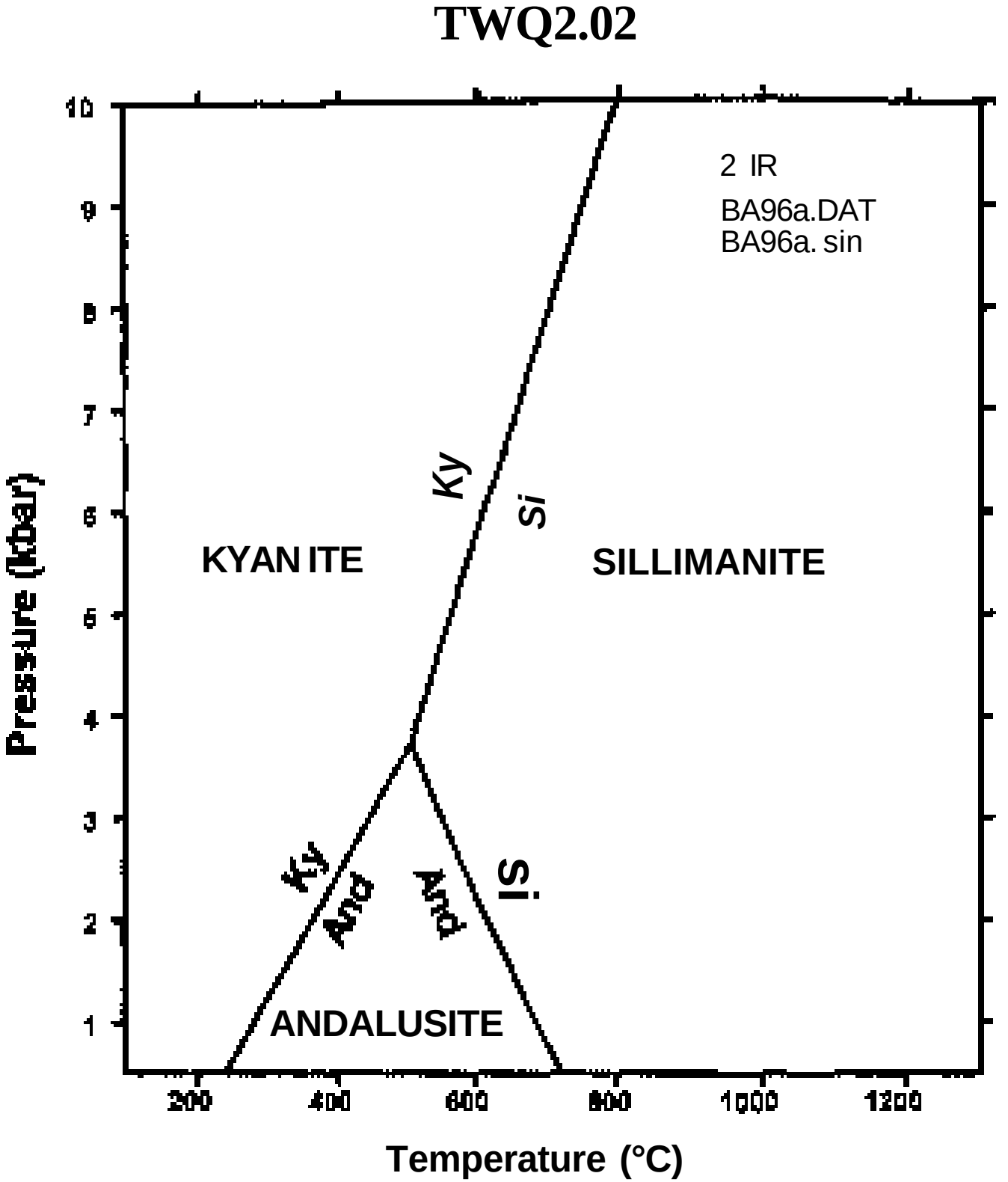
Exclusive Analysis

——Results include only 2 independent reactions——

Tot Ints	# Used	Yavg	Ydev	Xavg	Xdev
6	1	7842. 53	0. 00	509. 60	0. 00 excluding Si
6	1	7842.53	0. 00	509.60	0. 00 excluding aQz
6	2	7403.78	1.75	507. 43	0.10 excluding Gr
6	2	7403.78	1.75	507. 43	0.10 excluding An
6	2	7646.98	0. 96	494.19	0.05 excluding Alm
6	0	0.00	0 .00	0.00	0.00 excluding Ms
6	2	7646. 98	0. 96	494.19	0.05 excluding Ann
6	0	0.00	0. 00	0. 00	0.00 excluding Phi
6	0	0.00	0. 00	0. 00	0.00 excluding Py

Table 3 WEBINVEQ results for Sample No R9 124

INPUT DATA			
grossular	Activity 1	Uncertainty 1	
pyrope	Activity 1	Uncertainty 1	
almandine	Activity 1	Uncertainty 1	
Garnet Model	XCa 0 030	XMg 0 193	XFe 0 649
sillimanite	Activity 1	Uncertainty 1	
muscovite	Activity 1	Uncertainty 1	
White Mica Model	XK 0 650	XNa 0 349	XAl 0 874
phlogopite	Activity 1	Uncertainty 1	
annite	Activity 1	Uncertainty 1	
Biotite Model	M3 XMg 0 559	M3XFe 0 ?49	M3XTi 0 023
	AXK 0 783	OHXOH 1 00	
anorthite	Activity 1	Uncertainty 1	
Plagioclase Model	XAn 0 080	XAb 0 916	XOr 0 004
a quartz	Activ ty 1	Uncertainty 1	
		RESULTS	
Temperature	507 C	Pressure	7786 bars
Temperature variance	819 757 deg	Pressure variance	489758 bars
P T Covariance	14634 9 degree bars	Sum of squares of residuals	0 0787545 kJ
Number of equations	9	Number of unknowns	6
End member	Actual mu (kJ)	Best f t mu (kJ)	Error (kJ)
phlogopite	6476 898	6476 897	0 001
almand ne	5558 483	5558 558	0 074
grossular	6899 718	6899 690	0 028
muscovite	6202 275	6202 351	0 076
pyrope	6539 634	6539 636	0 001
a quartz	940 052	939 948	0 104
annite	5495 747	5495 673	0 074
s llıman te	2662 480	2662 272	0 208
anorth te	-4388 243	-4388 327	0 084



Fi g .1. *Phase diagram of the andalusite, kyanite and sillimanite using TWQ2 . 02*

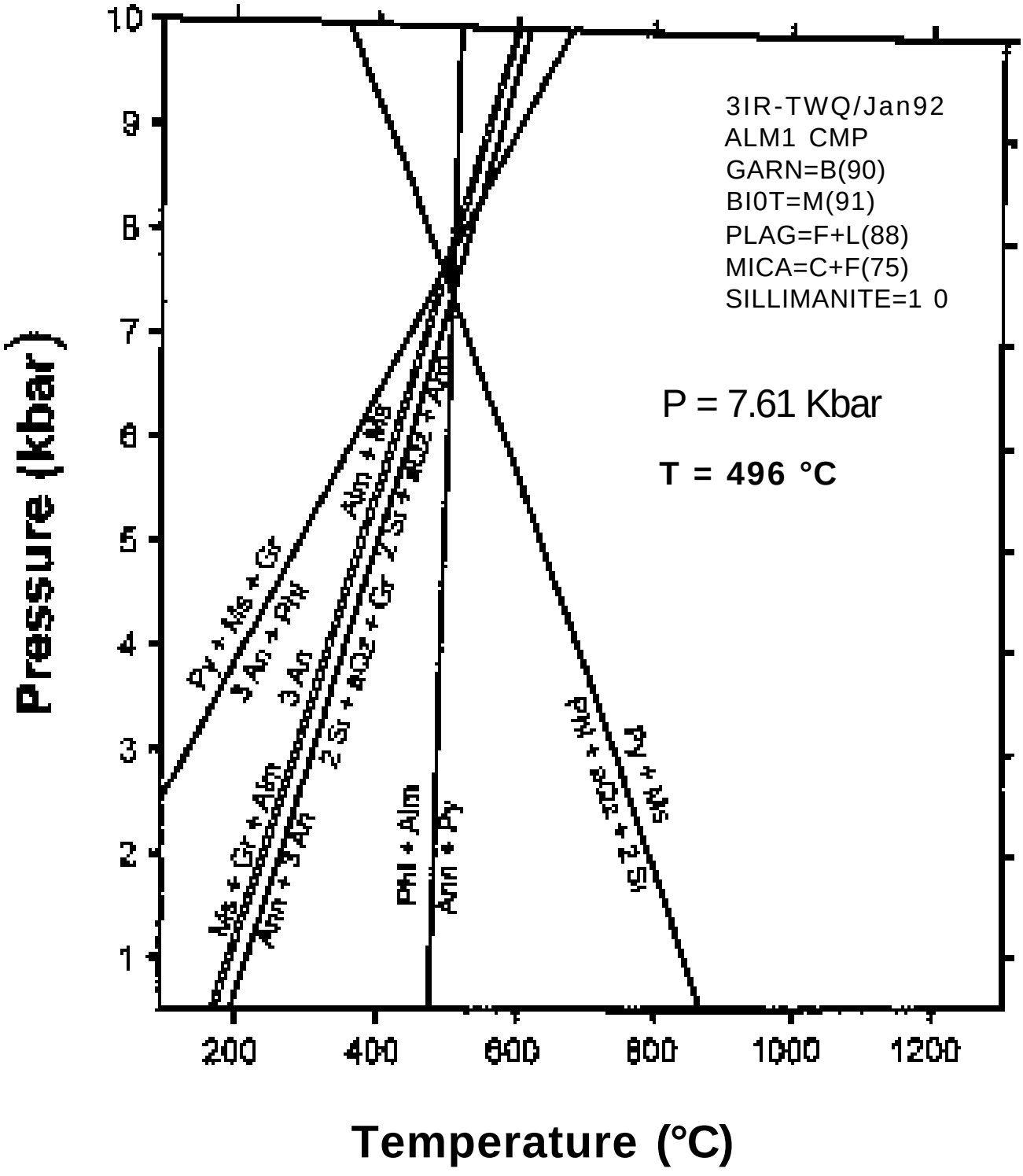
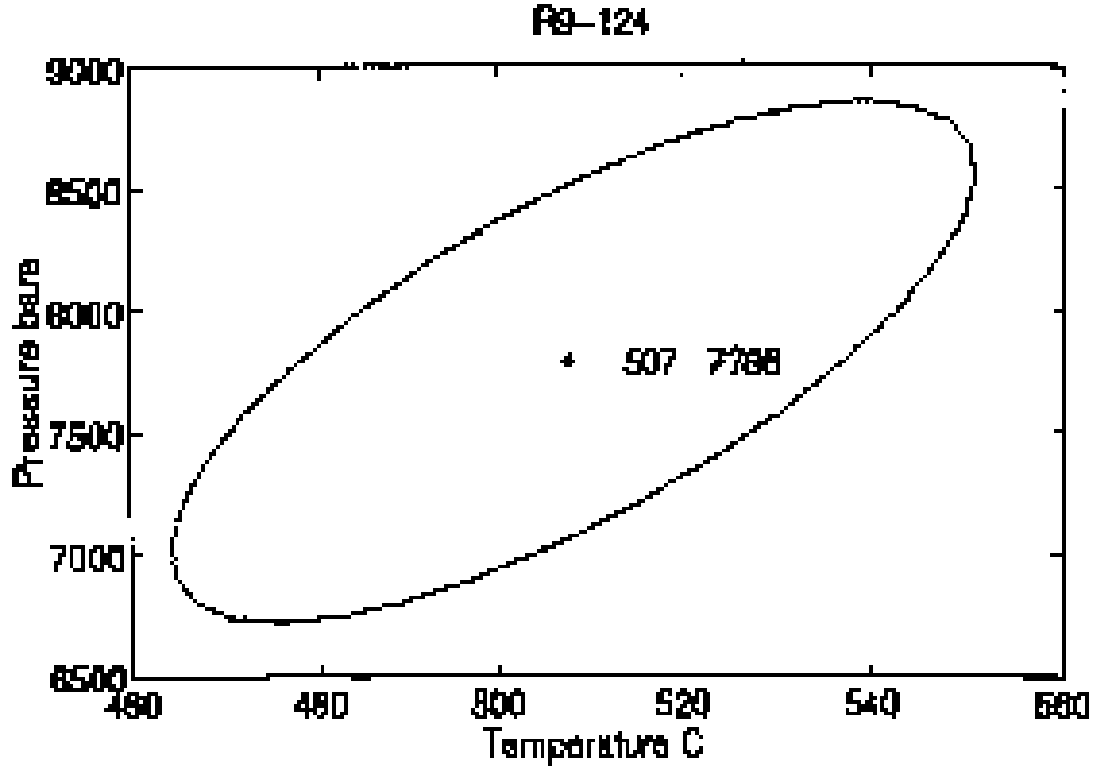


Fig .*2. Result obtained by TWQ1. 02 on sample no. R9 - 124 from Almora crystallines (garnet mica schist; sample location :right bank of Eastern Nyar, Marora village).*



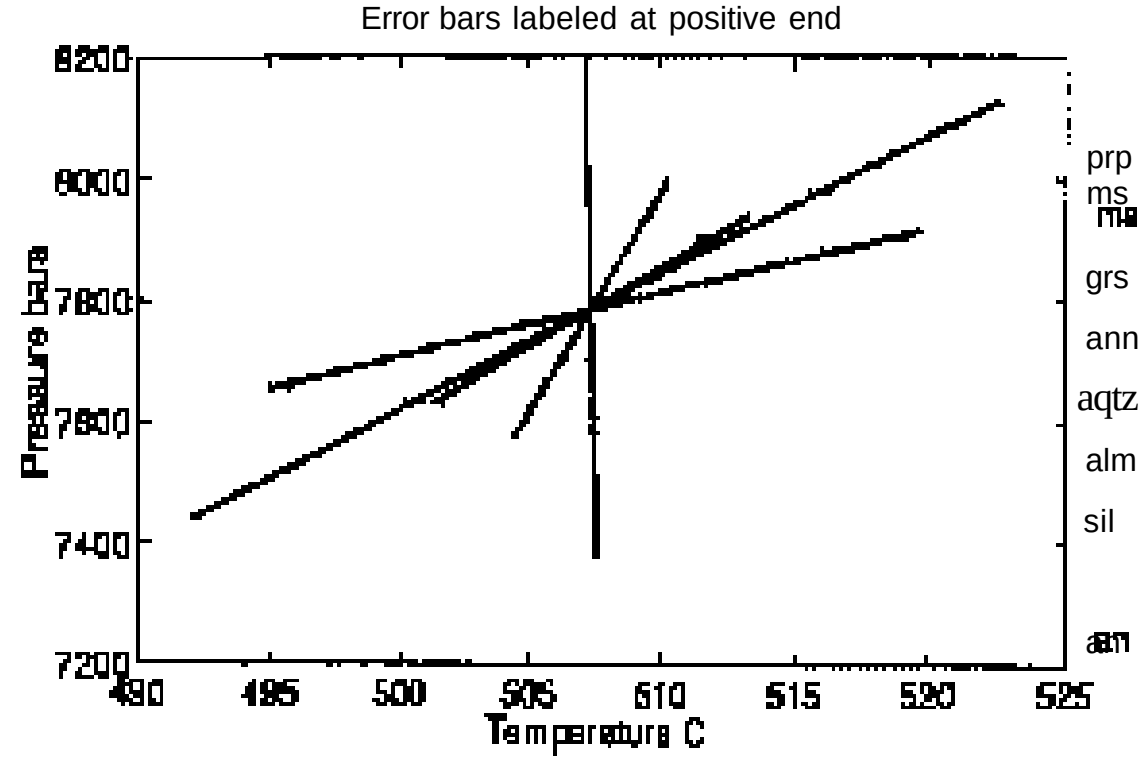


Fig.3. *WEB1NVEQ results for sample no. R9-124 using TWQ1. 02.*

Conclusions

In this paper review of computer Programs TWQ, WEBINVEQ and THERMOCALC is made with examples and applications. Some test runs are generated for demonstrating use of these computer programs along with P- T estimates done on the Dudatoli - Almora crystallines, Garhwal -Kumaon Lesser Himalaya.

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