Universität Salzburg
Fachbereich Geographie, Geologie, Mineralogie
Abteilung Mineralogie und Materialwissenschaften

Ao.Univ.-Prof. Dr. Edgar Dachs

Hellbrunnerstrasse 34/III
A-5020 Salzburg

Tel. +43-662-8044-5439
Fax +43-662-8044-622
email: edgar.dachs@sbg.ac.at
http://www.uni-salzburg.at/ggm

PET: Petrological Elementary Tools for Mathematica

Abstract

PET is a Mathematica package that supplies elementary tools for fulfilling various petrological tasks. Among these are mineral formula calculation (including nomenclature for amphibole according to the IMA sheme), calculation of mineral equilibria from internally consistent thermodynamic data sets (Berman or Holland and Powell), calculation of single equilibrium geothermobarometers (25 of the most common thermometers, 10 barometers), access to the thermodynamic functions of a particular phase and to activity models of various solid solutions, projection of the composition of a phase into a user-defined space and analysis of metamorphic assemblages by means of matrix methods. A major advantage of PET compared to already existing software is its wide range of applicability and flexibility, because PET tools can be easily grouped together and combined with Mathematica built-in functions in order to fulfill specific user-defined tasks.

Key Words: Thermodynamic calculations, Internally consistent thermodynamic data sets, Geothermometers, Geobarometers, Mineral formula calculation, Amphibole classification, Analysis of metamorphic assemblages

Introduction

An increasing number of software packages are becoming available for solving petrological problems. Most of these programs have been designed to perform specific tasks. These include PASFORM (Bjerg and others, 1995), HYPER-FORM (Bjerg and others, 1992), MINTAB (Rock and Caroll, 1990), MINFILE (Affifi and Essene, 1988), MINSORT (Petrakakis and Dietrich, 1985), as examples of general mineral formulae calculation programs, without mentioning the numerous applications for e.g. amphibole. Another class of software performs multiequilibrium calculations with internally consistent thermodynamic data sets (e.g.; TWQ, Berman, 1991; THERMOCALC, Holland and Powell, 1990). Geothermobarometry based on single equilibria calibrations is available through the softwares GPT for metapelites (Reche and Martinez, 1996), PTMAFIC for metabasites (Soto and Soto, 1995), BGT for garnet-biotite thermometer (Rao, 1995), SOLVCALC for feldspar thermometry (Wen and Nekvasil, 1994), PTOXY; a selection of 9 thermometers and 7 barometers (Nasir, 1994), and THERMOBAROMETRY, included in the program package of Spear and others (1991). Analysis of metamorphic assemblages with matrix methods can be performed with the programs MULTI and SVDMOD of Fisher (1989) and projections of mineral compositions for portraying phase relations in various types of diagrams with for instance TETPLOT (Spear et al., 1991), METPET (Ball and Robin, 1990), or ACF (Rock and Caroll, 1989). PET, the software presented here, provides a wide range of petrological elementary tools in one package, combining features of the programs mentioned above, using Mathematica (Wolfram, 1991). In its present form, it performs mineral formula calculation (including nomenclature for amphibole according to the IMA recommendations), calculation of mineral equilibria from internally consistent thermodynamic data sets (Berman 1988, Holland and Powell 1990), calculation of single equilibrium geothermobarometers (25 thermometers, 10 barometers), access to thermodynamic functions of a phase and to activity models of various solid solutions, projection of the composition of a phase into a user-defined space (numerically and symbolically), and analysis of metamorphic assemblages by means of matrix methods.

Installation of PET

PET was developed under Mathematica 2.2 (Wolfram, 1991) on a NeXT computer and also tested under WINDOWS on a DOS machine. It consists of 16 files containing Mathematica programs, 6 data files, a documentation file, and a file "examples" (see Appendix). To run PET, the Mathematica program is required, then download PET files from:

http://www.users.sbg.ac.at/~dachs

Assuming that the PET files reside onto your harddisk in a directory called PET, the Mathematica input:

```
SetDirectory["/PET"];

DeclarePackage["DEFDAT`",{"DatasetType","PET"}];

DatasetType[ ];
```

sets the current directory to /PET (note that a backslash has to be used on DOS mashines), such that Mathematica can find the PET files (first line), declares the functions DatasetType and PET that are used to define other functions (second line) and then loads PET with its default settings (Berman data set, functions for P-T type calculations) by calling DatasetType (third line, which can be modified using options). The above three lines have to be run once starting each PET application. If the type of calculation, or the thermodynamic data set need to be changed during a PET application, it is neccesary to quit Mathematica and restart.

Program description

Little Mathematica experinece of lists and functions is required to use the PET functions and to group them together in order to cover specific user-defined needs. Each function is associated with an online help-text, describing its usage, possible options, and also supplying one or more examples, which can be called with

FunctionName::usage

(Text written in italic indicates input-text for Mathematica throughout. These are definitions of lists or call to functions; results returned by functions are shown as normal text). PET functions may be grouped into general functions, fluid related functions and functions that calculate activity models of minerals. Some of these functions accept options that have predefined values which the user can change by applying the usual Mathematica syntax:

FunctionName[parameters, option -> value].
To see predefined values of options use:
Options[FunctionName].

General functions

PET functions that fulfill general petrological tasks are summarized in alphabetical order below.

CalcFormula

CalcFormula["filename"] calculates formula units of minerals and other mineral-chemical parameters such as site and mole fractions, and ideal mixing on site activities of phase components from wt% of oxides stored in the data file "filename" (ASCII format). A file named "hs78b", containing analyses of garnet, biotite, plagioclase and phengite from sample 78B of Hodges and Spear, (1982) is shown as an example below. Each analysis in this file (created by some editor) consists of a label, an abbreviation for that mineral followed by wt% of oxides, which may be given in any order.

Label	Mineral	SiO2	Al2O3	TiO2	MgO	FeO	MnO	CaO	Na2O	K2O
1	bt	36.31	19.74	1.43	10.04	18.35	0.12	0.11	0.28	7.9
2	wm	47.49	35.84	0.43	0.48	0.74	0	0.07	1.78	8.29
3	grt	38.53	21.85	0	2.3	33.77	4.86	0.87	0	0
4	plag	65.19	21.21	0	0	0	0	2.65	10.95	0.11

Available oxides in PET are:
Al2O3, BaO, BeO, B2O3, CaO, CeO2, Ce2O3, Cl, CoO, CO2, Cr2O3, Cs2O, CuO, Dy2O3, Er2O3, Eu2O3, F, FeO, Fe2O3, Gd2O3, HfO2, H2O, K2O, La2O3, Li2O, Lu2O3, MgO, MnO, MnO2, Mn3O4, Na2O, Nb2O5, Nd2O3, NiO, PbO, Pr2O3, P2O5, Rb2O, S, Sc2O3, SiO2, Sm2O3, SnO, SO3, SrO, Ta2O5, ThO2, TiO2, UO2, V2O3.Y2O3, ZnO, ZrO2.

For the usual rock-forming minerals, CalcFormula uses a predefined (anhydrous) oxygen basis in the formula calculation and recognizes such minerals by the following abbreviations (given in parentheses):

Alumosilicate (alsi, 5 O), amphibole (amph, 23 O), biotite (bt, 11 O), calcite (cc, 1 O), chlorite (chl, 14 O), chloritoid (ctd, 6 O), clinopyroxene (cpx, 6 O), cordierite (crd, 8), dolomite (dol, 2 O), garnet (grt, 12 O), ilmenite (fetiox, 3 O), kfeldspar (kfsp, 8 O), orthopyroxene (opx, 6 O), olivine (ol, 4 O), plagioclase (plag, 8 O), sapphirine (saph, 20 O), sphene (sphen, 5 O), spinel (spin, 4 O), staurolite (stau, 46 O), talc (talc, 11 O), white mica (wm, 11 O) and zoisite/epidote (zoep, 12.5 O).

It is also possible to process an analysis with a user-defined number of oxygens per formula unit. Fe3+ recalculation is carried out by default for pyroxene, garnet, spinel, chloritoid, sapphirine and ilmenite according to Droop (1987), and for amphibole following Leake and others (1997). For amphibole, the Fe3+ value calculated is the mean of minimum and maximum ferric estimates. However, the user can decide if this default return value is changed to the minimum or maximum Fe3+ estimate. Fe3+ recalculation and site fraction calculations for amphibole can also be performed according to Holland and Blundy (1994). Nomenclature for amphibole follows Leake and others (1997).

The results of CalcFormula:

```
{{mineral, label, SiO2, Al2O3, TiO2, MgO, FeO, MnO, CaO,Na2O, K2O, total}, {{bt, 1.,
2.7449, 1.7587, 0.08129, 1.1315, 1.1601, 0.007684, 0.008909, 0.04104, 0.7619, 94.28, {{{Al-
IV,Al-VI,Sum(cat),Sum(Ok),Sum(A)},
{XSi(T1),XAl(T1),XAl(M1),XFe2(M1),XMg(M1),XFe3(M1),XFe2(M2),XMg(M2),XVac(
M2)}}, {{1.2551, 0.5036, 7.696, 2.8841, 0.8118}, {0.3724, 0.6276, 0.25179, 0.357, 0.3482,
0, 0.4461, 0.4351, 0.11588}}}, {{{xfebt, xmgbt, xtibt, xalvibt, xkbt, xohbt}, {0.4022, 0.3923,
0.028186, 0.1746, 0.9385, 1.}}, {{ann, phl, sid, east}, {0.0405, 0.03757, 0.04813,
0.04578}}}}, {analogous lists for wm, grt and plag not shown}}
```

are stored as Mathematica list in the file "filename.fu" ("hs78b.fu" in this case) and are used by other functionssuch as ExtractSampleDat or CalcThermoBaro. They can be transformed to usual table format with the PET function MakeAnalysisTable["filename"].

CalcRea

CalcRea[rea, "filename"] calculates equilibrium data of reactions with the current thermodynamic data set (Berman 1988, or Holland and Powell 1990) for the desired diagram type (PT, TXCO2, oxygen buffer reactions, or redox reactions) using default starting and end values and predefined step sizes. rea is a Mathematica list defining the reaction(s) to be calculated and activities to be used. Taking the reaction muscovite + quartz = sanidine + kyanite + H2O as an example, this list has the form:

```
rea = {{{1. ms, 1. qza, -1. san, -1. ky, -1. h2o},{1,1,1,1,1}}},
```

and can be created with the PET function MakeRea before calling CalcRea by:

```
phases = {ms, qza, san, ky, h2o};

rea = MakeRea[phases];
```

In PET, phase components are defined by unique abbreviations such as ms for muscovite (available phases and their abbreviations can be viewed by the PET function MinList). The first line above is a user-defined list named phases consisting of the elements ms, qza, san, ky, and h2o. In the second line, the list phases is passed to the PET function MakeRea, which calculates the reaction stoichiometry for the elements in phases (using unit activities as default), assigning its result to the variable rea, as shown above. This is then used in the call to CalcRea:

```
result = CalcRea[rea, "filename"];
```

The results of CalcRea (see Example 15) are stored as list in the file "filename.ptx" and can be plotted with the PET function PlotRea.

It is also possible to use CalcRea in combination with activity models to calculate mineral equilibria for specific samples from their mineral-chemical data.

CalcReaIntersection

CalcReaIntersection[result] can be used to calculate intersections of reactions from the results returned by CalcRea.

CalcThermobaro

CalcThermoBaro[{gtb1, gtb2, ...}, "inputfile", "outputfile"] calculates various geothermobarometers (gtb's; see CalcThermoBaro::usage which gtb's are available). Each gtb in the list {gtb1, gtb2, ...} has the form:

{{min1, min2, ...}, {min, max, step}},

where {min1, min2, ...} is a list of the mineral abbreviations forming the gtb, e.g. {grt, bt} for the garnet-biotite geothermometer, and the list {min, max, step} defines the pressure range and interval for which temperatures are calculated in the case of a geothermometer, and vice versa for geobarometers. "inputfile" must have been created earlier with CalcFormula["inputfile"] and may contain analyses for more than one pair of e.g. garnet and biotite (in this case, analyses are grouped together in order of appearance, 1.grt with 1.bt, 2.grt with 2.bt, etc. The result of CalcThermoBaro is written to "outputfile.ptx" for later use and is a list of the form:

{{{min1, min2, ...},{inputfile, {lnKD = some value, GtbCalibration = reference of the calibration used}}, {pairs of calculated T-P}}}.

Taking the file "hs78b" as an example and assuming that formulae have been already calculated with CalcFormula["hs78b"],

result = CalcThermoBaro[{{{grt,bt},{2000,6000,1000}}},"hs78b","test"]

would calculate the garnet-biotite geothermometer from data read from the file "hs78b.fu" between 2 and 6 kbar in a 1 kbar interval, producing:

{{{grt, bt}, {hs78b, {lnKD = -2.08362, GrtBtCalibration = Kleemann & Reinhardt (1994), eq.(5), (19), with Berman 1990 garnet model}}, {{509.522, 2000}, {512.206, 3000}, {514.89, 4000}, {517.574, 5000}, {520.258, 6000}}}}.

This is assigned to the variable result and stored in the file "test.ptx".

For most gtb's, there are several calibrations available that can be viewed with FunctionName::usage (e.g. GrtBt::usage). The program returns the latest version by default. However, the user can choose the calibration most appropriate for their purposes. The result of CalcThermoBaro can be plotted with PlotRea and intersections of geothermometers with geobarometers can be calculated with CalcReaIntersection. The file "gtb", delivered with PET, is an arbitrary collection of analyses that allow it to test all gtb's.

DatasetType

selects the thermodynamic dataset to be used and the diagram type for calculations. This function has two options, Dataset and Type , which have the default settings Dataset ->Berman88 and Type->PT. If called in the form DatasetType[ ], the Berman (1988) data set (extracted from the file jan92.rgb, TWQ, version 1.0) and functions for P-T calculations are automatically loaded. Alternatively, if DatasetType is called with DatasetType[Dataset->HollandPowell], the Holland and Powell (1990) data set can be loaded (as used by THERMOCALC, version 2.3). The option Type accepts the alternative values TXCO2, O2Buffer (reactions with only O2 as gas species), Redox (equilibria with only H2 (and H2O) as gas species), and Chemography. This function must be called **once** at the beginning of each PET session.

DeletePhase

deletes chemical data of a phase from the file "CHEM.M" that was inserted earlier with InsertPhase (see below). The chemical data of phases stored in this file (all phases as in the Holland and Powell data set plus compounds like FeO, MgO, CaO, etc., plus user-defined phases inserted with InsertPhase) are used by PET for chemography tasks (in this case DatasetType must have been called with the option DatasetType[Type->Chemography]). This way, the user has the opportunity to use their own mineral-chemical data of a sample for e.g. projection purposes or mass balance calculations.

Dgr

calculates dGR of a reaction as a function of P and T (and XCO2 or XH2 if DatasetType was called with the option Type->XCO2 or Type->Redox).

ExtractMinDat

EctractMinDat[mineral_abbreviation, parameter, "filename"] can be used to extract a mineralchemical parameter of a phase (defined by mineral_abbreviation) from the file "filename.fu", created before with CalcFormula. If there are several analyses of that phase in "filename.fu", ExtractMinDat returns a list of the parameter values. This function is useful, if a plot of parameter1 versus parameter2 of the same or different phases shall be created (e.g. with the Mathematica built-in functions ListPlot or MultipleListPlot). If, as an example, Al_IV versus Al_VI of white mica shall be plotted, this is achieved with:

```
alvi = ExtractMinDat[wm, AlVI, "filename"];
aliv = ExtractMindat[wm, AlIV, "filename"];
ListPlot[Transpose[{alvi,aliv}]]
```

ExtractSampleDat

ExtractSampleDat["filename",{list of phase-components}] extracts sample data (mineral-chemical parameters such as mole fractions required to calculate activity models) from the file "filename.fu" and returns the list phases for MakeRea, such that data of a specific sample can be used in PTX calculations. Assume, as an example, that you wish to calculate the garnet - biotite geothermometer with an internally consistent data set from the mineralchemical data stored in the file "hs78b.fu", produced with CalcFormula["hs78b"]. The Mathematica input:

```
phases = ExtractSampleDat["hs78b",{ann,phl,alm,py}]
```

assignes the list

```
{{ann, phl, alm, py}, {am, am, am, am}}
```

to the variable phases, which, when passed to rea = MakeRea[phases] to calculate the reaction stoichiometry between the phase components annite, phlogopite, almandine and pyrope, results in the following output assigned to the variable rea:

```
{{{1. ann, -1. phl, -1. alm, 1. py}, {am, am, am, am}}}.
```

The abbreviation "am" in the the list {am, am, am, am} stands for activity model and indicates that for each corresponding element in {1. ann, -1. phl, -1. alm, 1. py} an activity model will be used by CalcRea. The required mole fractions have been copied by ExtractSampleDat into the file "SAMPLE.DAT" shown below:

```
{{{xfegt, xmggt, xcagt, xmngt}, {0.7691, 0.09338, 0.025386, 0.11211}}, {{xfebt, xmgbt,
xtibt, xalvibt, xkbt, xohbt}, {0.4022, 0.3923, 0.028186, 0.1746, 0.9385, 1.}}}
```

The mathematica input:

```
result = CalcRea[rea, "test"]
```

then calculates the garnet-biotite geothermometer for the sample 78B with the default activity models and predefined settings, by reading the data from the file "SAMPLE.DAT". If a phase component in {list of phase-components} is not found by ExtractSampleDat in the file "hs78b.fu" (e.g. quartz), its activity is automatically set to unity.

G

G[min, P (bar), T (K)] calculates the Gibbs Free Energy function of the phase min at P and T with the current thermodynamic data set (min is the abbreviation of that phase as viewed by MinList, e.g. ms for muscovite). With the option ReturnValue, the user has access to other thermodynamic functions of a phase: ReturnValue->Hint returns Int cp dT, ReturnValue->Sint returns Int cp/T dT, ReturnValue->Vint returns Int V dP (only solids), ReturnValue->V returns the volume (only solids), and ReturnValue->Cp returns cp of the phase min.

GetRea

GetRea["filename"] reads equilibrium data from the file "filename", calculated earlier with CalcRea.

GOrd

calculates order/disorder related parameters of relevant phases (see Berman, 1988, and Holland and Powell, 1990, for more details on which phases exhibit order/disorder phenomena). For albite, parameters are calculated according to Salje and others (1985).

InsertPhase

InsertPhase[mineral_abbreviation, user-defined_abbreviation, user-defined_phasename, "filename"] inserts chemical data of a mineral into the file "CHEM.M", such that these data can be used for chemographic purposes, for instance calculation of reaction relations for the mineral assemblage of a sample (in this case DatasetType must have been called with the option DatasetType[Type->Chemography]). The parameter mineral_abbreviation must be any cited above under CalcFormula (e.g. bt for biotite) and chemical data for that phase are read from the file "filename.fu" and stored with user-defined_abbreviation, and user-defined_phasename in the file "CHEM.M". If, as an example, the data of biotite stored in the file "hs78b.fu" is required for chemography tasks, this is achieved with:

```
InsertPhase[bt, bths78b, BIOTITE_HS78B, "hs78b"]
```

MakeAnalysisTable

MakeAnalysisTable["filename"] stores analyses and calculated formula units in table format (e.g. for import into a text program) in the file "filename.tab" (see Example 23), by combining wt% from the file "filename", with formula units from the file "filename.fu", as created with CalcFormula["filename"]. The options MakeAnalysisTableDigits and MakeAnalysisTableSplit determine the number of digits in the final table (default 3) and the number of analyses in successive columns, before the file is split into separate parts (default 10).

MakeRea

MakeRea[phases] calculates a set of linearly independent reactions that can be written among the phase components specified in the list:

```
phases = {min1, min2, min3, ...};
```

where each element in this list has to be a phase abbreviation as viewed by MinList (e.g. ms for muscovite). The output of MakeRea is the required input for CalcRea. MakeRea also accepts an input-list of the form:

```
phases = {{min1, min2, min3, ...},{act1, act2, act3, ...}};
```

allowing the specification of fixed activities for each phase component (otherwise unit activities are inserted by default). The sequence

```
phases = {ky, sil, and};
```

```
rea = MakeRea[phases]
```

for example, calculates two reactions:

```
{{{-1. ky, 1. and}, {1., 1.}}, {{-1. ky, 1. sil}, {1., 1.}}}
```

assigning this list to the variable rea.

MakeAllRea

MakeAllRea[phases] calculates all possible reactions that can be written among the phase components specified in the list phases, and not just a set of linearly independent ones as with MakeRea. By changing the default value of the option MakeAllReaMode, it is possible to analyse metamorphic assemblages following the principles discussed by Fisher (1989), by determining the singular value decomposition of their composition matrix, and by calculating mass balance relations (e.g. Whitney and others, 1995).

MinDat

MinDat[min] returns a 30-element list containing the thermodynamic and chemical data of the phase min from the current thermodynamic data set. The option AnnDat can be used to switch to annite standard data according to Dachs (1994a) or Dachs and Benisek (1995).

MinList

MinList[ ] returns a list of the available phases in the current thermodynamic data set and their abbreviations in PET. The name of a phase is written in uppercase, followed by the PET abbreviation in lowercase, for instance:

```
{MUSCOVITE, ms}
```

O2Buffers

O2buffers[P (bar), T (K)] calculates logfO2 at P and T for various oxygen buffers from emf-data (O'Neill and Pownceby, 1993, O'Neill, 1987, 1988). The option Buffer is set by default to NNO,(causing return of logfO2 for the NiNiO buffer), but accepts the alternative values QFM, QFI, WM, WI, MI, CCO and CuCu2O, in which case the logfO2 of the quartz-fayalite-magnetite, quartz-fayalite-iron, wuestite-magnetite, wuestite-iron, magnetite-iron, Co-CoO, and Cu-Cu2O buffers is calculated.

PlotRea

is used to plot equilibrium data calculated earlier with CalcRea. PlotRea uses the Mathematica built-in function ListPlot and connects data points by a line. The plot style of the graphic object returned by PlotRea can be modified with the Mathematica function Show and associated options.

Projection

Projection[min,{{projection points},{space}}] allows the projection of a mineral min from a user-defined list {projection points} into a user-defined {space}. The function performs a coordinate transformation from old components (chemical elements) into new components defined by {{projection points},{space}} (see Spear, 1993, chapter 5 for more details). To use this function, the Mathematica session must be started with DatasetType[Type->Chemography], which makes phases of the file "CHEM.M" available. If, as a simple example, tremolite (abbreviation tr) shall be projected into the triangle SiO2-CaO-MgO, this is achieved with:

```
result = Projection[tr, {{h2o},{sio2,cao,mgo}}]
```

returning the coordinates:

```
{8/15, 2/15, 1/3}
```

ProjectionSymbolic

One of the most powerful features of Mathematica is the possibility to perform calculations symbolically. ProjectionSymbolic[{{projection points},{space}}] makes use of this ability and calculates projections symbolically from a user-defined list {projection points} into a user-defined {space} (the projection is expressed in terms of elements Si, Al, Fe, etc.). To calculate the AFM projection for instance, the required Mathematica input would be:

```
result = ProjectionSymbolic[{{qza,ms,h2o},{al2o3,feo,mgo}}]
```

SaveRea

SaveRea[rea, "filename"] can be used to save calculated equilibrium data or reaction stoichiometries (everything assigned to rea) to the file "filename".

SelectRea

SelectRea[{paragenesis}, rea] selects all those reactions from a list of reactions rea that contain the phases defined in the list {paragenesis} (rea must have been created with MakeAllRea or MakeRea). This function is useful if, from a list of reactions, those containing special phases need to be filtered.

SelectIncompRea

SelectIncompRea[{paragenesis1}, {paragenesis2}, rea] searches the list rea (containing reaction stoichiometries calculated with MakeAllRea or MakeRea) to find those reactions where a mass balance exists between the lists {paragenesis1} and {paragenesis2}, e.g. reactions with {paragenesis1} on one side of the reaction equation, and {paragenesis2} on the other. This function can be used to analyse metamorphic assemblages and find incompatibilities between user-defined parageneses (parageneses that intersect in composition space and cannot have equilibrated under the same conditions; see Fisher, 1989).

TransformDatFile

TransformDatFile["microprobe-filename","filename"] transforms a microprobe results file (oxide weight %) into the file "filename" that has the reqired structure to be readable for CalcFormula. It was written for a JEOL-JX 8600 microprobe and can be adapted to other data file structures with some Mathematica experience. The user only need edit the file "microprobe-filename" (containing results in ASCII format, summarized as oxide wt%) modifying analyses labels to a form that they contain the correct abbreviation, as recognized by CalcFormula (e.g. grt for garnet). Microprobe data can thus be processed without retyping the analyses. The file "hs78b.emp" is an example of a transformable microprobe data file.

Fluid related functions

PET supplies functions that calculate fluid properties such as volume, fugacity or activity. Pure fluid properties can be calculated for H2O, CO2, H2, and H2O-CO2 mixed fluid properties are available according to Kerrick and Jacobs (1981). The H2O-H2 system is calculated with the MRK of Holloway (1977) using a and b parameters for H2O from Holloway (1977) and for H2 published in Connolly and Caesare (1993).

Activity models for minerals

Available activity models for solid solutions in PET are those for biotite, clinopyroxene, feldspar, garnet and white mica and are used by CalcRea, if the list in the call to CalcRea, specifying the reactions, contains "am" in the sublist defining the activities. In this case, the required mole fractions of that phase component are read from the file "SAMPLE.DAT" (see ExtractSampleDat for more details). Activity of biotite phase components can be calculated by default according to McMullin (1991), or with Margules parameters according to Benisek and others (1996) and Circone □and Navrotsky (1992). Activities in sodic, disordered C2/c clinopyroxene are calculated following Holland (1990). For feldspar, activities of phase components are available according to Elkins and Grove (1990), Lindsley and Nekvasil (1989), Fuhrman and Lindsley (1988), Nekvasil and Burnham (1987), Green and Usdansky (1986) and Ghiorso (1984). By default, the calculated model is that of Elkins andGrove (1990). Available garnet activity models are those from Mukhopadhyay and others (1997), Berman and Aranovich (1996), Ganguly and others (1996), Dachs (1994b), Berman (1990) and Ganguly and Saxena (1984). If PET has been started with its default setting, loading the Berman data set, garnet activities are automatically returned according to Berman (1990). Activities of white mica phase components are calculated according to Chatterjee and Froese (1975).

Application examples

A selection of some examples from the file "examples", demonstrating the use of PET functions in various applications, follows below (example numbers are not in continuous order, but as in the file "examples"). If not stated otherwise, all these examples assume that the above three lines have already been run. Required input by the user is shown, as above, in italic, calculated results as normal text (intermediate results are shown for input-lines that do not end with a semicolon). Some PET functions write text to the screen during calculation, which is not shown here.

Example 2: Show a list of all available PET functions.

```
PET::usage
```

Example 5: Use the PET function G to plot the Gibbs Free Energy surface of sillimanite for pressures between 1 and 10000 bar, and temperatures between 500 and 1000 K. Use the Mathematica built-in function Plot3D to make a threedimensional plot.

```
plot = Plot3D[G[sil,p,t],{p,1,10000},{t,500,1000}, AxesLabel->{"P(bar)","T(K)"," "}];
```

Example 6: Use the PET function G to calculate ò cp dT of quartz for temperatures between 300 and 1000 K (1 bar), and the Mathematica built-in function Plot to plot the results.

```
plot = Plot[G[qza,1,t,ReturnValue->Hint],{t,300,1000}, AxesLabel->{"T(K)","H(T)-H(298)"}];
```

The inflection point of the curve at 848 K is due to the a/b-quartz phase transition (compare Chatterjee, 1991, Fig. 2.2).

Example 10: Use the PET functions Aco2 and Ah2o to plot H2O- and CO2 activities in H2O - CO2 fluids at 4 kbar, 600 °C, and the Mathematica built-in functions Plot and Show to display the graph.

```
plot1=Plot[Aco2[4000, 873.15,xco2],{xco2,0,1},DisplayFunction->Identity];
plot2=Plot[Ah2o[4000, 873.15,1-xco2],{xco2,0,1},DisplayFunction->Identity];
Show[plot1,plot2,Frame->True,PlotRange->{{0,1},{0,1}}, FrameLabel-
>{"X(CO2)","A(H2O) or A(CO2)"},DisplayFunction->$DisplayFunction]
```

DisplayFunction->Identity causes that plot1 and plot2 are suppressed, only the combined plot is shown.

Example 12: Use the PET function GOrd to plot the order parameters Q and Qod for albite as function of temperature (Salje and others, 1985), and the Mathematica built-in functions Plot and Show to display the graph.

```
p1=Plot[GOrd[ab,1,t,1][[6]],{t,0,1300},DisplayFunction->Identity];
p2=Plot[GOrd[ab,1,t,1][[7]],{t,0,1300},DisplayFunction->Identity]; Show[p1,p2,Frame-
>True,PlotRange->{{0,1300},{0,1}}, FrameLabel->{"T(K)","Q(od) or Q"},DisplayFunction-
>$DisplayFunction]
```

Example 15: Use the PET functions MakeRea to calculate a reaction for the phases muscovite, quartz, sanidine, kyanite, water (adopting the default setting activity = 1 for all phases), CalcRea to calculate PT-data of the reaction found by MakeRea (setting Pstep to 250 and Pmax to 6000), and saving results to the file "test".

```
phases ={ms,qza,san,ky,h2o};
```

```
rea = MakeRea[phases];
```

```
result = CalcRea[rea,"test",Pstep->250,Pmax->6000]
```

```
{{{-1. ms, -1. qza, 1. san, 1. ky, 1. h2o}, {1., 1., 1., 1., 1.}, {{564.608, 500}, {586.185, 750},
{601.368, 1000}, {613.633, 1250}, {624.314, 1500}, {633.994, 1750}, {642.977, 2000},
{651.439, 2250}, {659.493, 2500}, {667.217, 2750}, {674.667, 3000}, {681.884, 3250},
{688.901, 3500}, {695.744, 3750}, {702.434, 4000}, {708.987, 4250}, {715.418, 4500},
{721.739, 4750}, {727.96, 5000}, {734.091, 5250}, {740.14, 5500}, {746.112, 5750},
{752.015, 6000}}}}
```

Example 18: Use the PET functions CalcFormula to calculate the formula units for the file "hs78b", ExtractSampleDat to extract mineral-chemical parameters for the phase components {ann, phl, alm, py, gr, an, qza, sil}, creating the required input-list for MakeRea, MakeRea to calculate a set of linearly independent reactions, SetOptions (Mathematica built-in) to change the default feldspar activity model of the function Afs to the calibration of Fuhrman & Lindsley, CalcRea to calculate P-T data of the reactions found by MakeRea, setting Pstep to 1000, PlotRea to plot the results, and CalcReaIntersection to calculate the intersection of the garnet-biotite geothermometer with the GASP barometer.

```
CalcFormula["hs78b"];
```

```
phases = ExtractSampleDat["hs78b",{ann,phl,alm,py,gr,an,qza,sil}]
```

```
rea = MakeRea[phases] SetOptions[Afs,AfsModel->FuhrmanLindsley]; result =
CalcRea[rea,"test",Pstep->1000]
```

```
plot = PlotRea[result]; CalcReaIntersection[result]
```

```
{{ann, phl, alm, py, gr, an, qza, sil}, {am, am, am, am, am, am, 1., 1.}}
```

```
{{{1. gr, -3. an, 1. qza, 2. sil}, {am, am, 1., 1.}}, {{1. ann, -1. phl, -1. alm, 1. py}, {am, am,
am, am}}}
```

```
{{{1. gr, -3. an, 1. qza, 2. sil}, {am, am, 1., 1.}, {{288.88, 500}, {341.821, 1500}, {394.51,
2500}, {446.92, 3500}, {499.013, 4500}, {550.752, 5500}, {602.103, 6500}, {653.036,
7500}, {703.527, 8500}, {753.556, 9500}}}, {{1. ann, -1. phl, -1. alm, 1. py}, {am, am, am,
am}, {{461.341, 500}, {466.225, 1500}, {471.091, 2500}, {475.939, 3500}, {480.77, 4500},
{485.582, 5500}, {490.377, 6500}, {495.153, 7500}, {499.912, 8500}, {504.652, 9500}}}}
```

```
{{4113.21, 478.904, {1, 2}}}
```

The calculated results shown above are created from the input statements in line two, three, five and seven (those missing a semicolon at the end), demonstrating equilibration of sample 78B at 4.1 kbar and 479 (C). The same calculation with the Holland and Powell data set yields 5.5 kbar and 467 (C).

Example 23: Use the PET functions CalcFormula to calculate mineral formulae for the microprobe data in the file "gtb", and MakeAnalysisTable to produce a table of the analyses.

```
CalcFormula["gtb"]; MakeAnalysisTable["gtb"];
```

Example 28: Use the PET functions CalcThermoBaro to calculate the garnet-biotite thermometer and the GASP barometer for the data file "hs78b", (using the default calibrations), storing results in the file "test", PlotRea to display the results, and CalcReaIntersection to calculate the intersection.

```
CalcFormula["hs78b"];
```

```
result = CalcThermoBaro[{{{grt,bt},{2000,10000,2000}}, {{grt,plag},
{400,600,25},sillimanite}},"hs78b","test"]
```

```
PlotRea[result];
```

```
CalcReaIntersection[result]
```

```
{{{grt, bt}, {gtb, {lnKD = -2.08361, GrtBtCalibration = Kleemann & Reinhardt (1994),
eq.(5), (19), with Berman 1990 garnet model}}, {{509.525, 2000}, {514.893, 4000},
{520.261, 6000}, {525.629, 8000}, {530.997, 10000}}}, {{grt, plag}, {gtb, {lnK = -1.62766,
GrtPlagCalibration = Koziol (1989), sillimanite}}, {{400, 3141.83}, {425, 3681.38}, {450,
4220.69}, {475, 4759.77}, {500, 5298.61}, {525, 5837.23}, {550, 6375.6}, {575, 6913.74},
{600, 7451.65}}}}
```

```
{{5718.9, 519.507, {1, 2}}}
```

Example 30: Start PET for chemography purposes and use the PET functions MakeAllRea to calculate all reactions for the hypothetical phases {qza, opm2, opm3, olm2, olm3}, (hypothetical example of Fisher, 1989) and SelectIncompRea to find incompatibilities.

```
DatasetType[Type->Chemography];
```

```
phases = {qza,opm2,opm3,olm2,olm3};
```

```
rea = MakeAllRea[phases]
```

```
SelectIncompRea[{opm3,olm3},{olm2,opm2,qza},rea]
```

```
{{-0.50129 olm2, 0.50178 olm3, 1. opm2, -1.0006 opm3}, {0.50456 olm2, 1. opm2, -2.0084
opm3, 0.50358 qza}, {1. olm2, -0.66667 olm3, -0.66667 opm2, 0.33333 qza}, {1. olm2, -
0.49886 olm3, -1.0019 opm3, 0.50065 qza}, {0.25171 olm3, 1. opm2, -1.5029 opm3, 0.25097
qza}}
```

```
{{0.50456 olm2, 1. opm2, -2.0084 opm3, 0.50358 qza}, {1. olm2, -0.49886 olm3, -1.0019
opm3, 0.50065 qza}}
```

This finds five possible reactions and two incompatibilities, as discussed by Fisher (1989). The statement DatasetType[Type->Chemography] causes that MakeAllRea now reads data from the file "CHEM.M" (the "phases" opm2, opm3, olm2 and olm3 have already been inserted). Note that MakeRea performs a singular value decomposition (SVD) on the composition matrix before calculating the reactions (using 0.01 as value for the option SVDLimit (see next example).

Example 31: Use the PET function MakeAllRea to perform a singular value decomposition of the composition matrix defined by the "phases" {qza,opm2,opm3,olm2,olm3}.

```
phases = {qza,opm2,opm3,olm2,olm3};
```

```
rea = MakeAllRea[phases,MakeAllReaMode->4,SVDLimit->0]
```

```
{4., 1, {7.94308, 0.88956, 0.17846, 0.00048, 0}, rest = two matrices not shown}
```

The first two elements in the list above are the rank of the composition matrix and the number of linearly independent reactions, followed by a list representing the SVD (diagonal elements of the matrix W in Fisher, 1985). The model composition matrix calculated from the SVD, and a matrix of the residuals (differences between composition and model matrix) is also returned, but not shown in this example. Because the element 0.00048 in the SVD is close to zero, the composition matrix defined by the "phases" {qza,opm2,opm3,olm2,olm3} is in fact close to a matrix of rank three, which is used by MakeRea when SVDLimit is set to e.g. 0.01 (the default setting), as shown by:

```
phases = {qza,opm2,opm3,olm2,olm3};
```

```
rea = MakeAllRea[phases,MakeAllReaMode->4,SVDLimit->0.01]
```

```
{3., 2, {7.94308, 0.889563, 0.178464, 0, 0}, rest = two matrices not shown}.
```

Example 39: Use the reversed equilibrium data of the reaction muscovite + quartz = sanidine + andalusite + H2O from Chatterjee and Johannes (1974) to extract dHoR and dSoR for that reaction (text enclosed by "(*" and "*)" is comment text). From the thermodynamic relation:

T T P - dHoR + T dSoR = ò dcpR dT - T Int (dcpR/T) dT + Int DVs dP + R T lnfH2O, 298 298 1 "hint" "sint" "vint" "rtlnfh2o"

it follows that if a data vector dv = hint - T sint + vint + rtlnfh2o is fitted against T, the slope is dSoR and the intercept is -dHoR. Starting PET with its default settings, the solution for this example is:

```
(* dat is a list of the equilibrium data *) dat = {{500, 560},{500,
540},{500,520},{1000,570},{1000,550},{2000,605},{2000,595},
{2000,590},{3000,640},{3000,630},{3000,620},{4000,670},{4000,660},{5000,705},
{5000,695},{5000,690}}; {p,t} = Transpose[dat]; (* p is a list of the pressures, t of the
temperatures *) t = t + 273.15; (* calculate Kelvin temperatures *)
```

```
(* hint is a list of the H-Integrals for each experimental P and T *)
hint=Map[G[and,#[[1]],#[[2]],ReturnValue->Hint]+G[san,#[[1]],#[[2]],ReturnValue->Hint]+
G[h2o,#[[1]],#[[2]],ReturnValue->Hint]-(G[ms,#[[1]],#[[2]],ReturnValue->Hint]+
G[qza,#[[1]],#[[2]],ReturnValue->Hint])&,Transpose[{p,t}]];
```

```
(* sint is a list of the S-Integrals for each experimental P and T *)
sint=Map[G[and,#[[1]],#[[2]],ReturnValue->Sint]+G[san,#[[1]],#[[2]],ReturnValue->Sint]+
G[h2o,#[[1]],#[[2]],ReturnValue->Sint]- (G[ms,#[[1]],#[[2]],ReturnValue->Sint]+
G[qza,#[[1]],#[[2]],ReturnValue->Sint])&,Transpose[{p,t}]];
```

```
(* vint is a list of the V-Integrals for each experimental P and T *)
vint=Map[G[and,#[[1]],#[[2]],ReturnValue->Vint]+G[san,#[[1]],#[[2]],ReturnValue->Vint]+
G[h2o,#[[1]],#[[2]],ReturnValue->Vint]-(G[ms,#[[1]],#[[2]],ReturnValue->Vint]+
G[qza,#[[1]],#[[2]],ReturnValue->Vint])&,Transpose[{p,t}]]; (* rtlnfh2o is a list of
RTlnf(H2O) for each experimental P and T *) rtlnfh2o=Map[8.3143 #[[2]]
Log[Fh2o[#[[1]],#[[2]]]]&,Transpose[{p,t}]]; (* dv is the data vector that should yield a
straight line when plotted against T *) dv = hint - t sint + vint + rtlnfh2o;
```

```
(* plot the data vector against T *) plot = ListPlot[Transpose[{t,dv}],AxesLabel-
>{"T(K)","dv"}];
```

```
(* fit the data: slope is DSoR, intercept is -DHoR *) fit = Fit[Transpose[{t,dv}],{1,x},x]
```

```
-101065. + 180.94 x
```

```
(* compare this to D reaction properties from the data set *) delta =
(MinDat[and]+MinDat[san]+MinDat[h2o])-(MinDat[ms]+MinDat[qza])
```

```
{95948.1, 174.694, plus other D reaction properties not shown}
```

Discussion

A selection of elementary petrological tasks solvable with PET has been presented above. A major advantage of PET is the wide range of possible applications and its flexibility, because functions can be easily grouped together to fulfill specific user-defined needs. Thus, it is possible to, for instance, process microprobe data to arrive at a geothermobarometric result without the user being forced to retype any analysis or intermediate result, or creating some related data files, as PET functions work hand in hand. Graphic objects created by PET can be brought to publication-ready standard utilysing Mathematica's built-in cababilities. However, the usage of PET is not restricted to purely scientific applications. The easy display of thermodynamic functions may be useful for teaching purposes. However, a disadvantage of PET compared to compiled programs is its lower computational speed. Equilibrium data, calculated with CalcRea for a lot of equilibria involving solids, have been tested against the results of TWQ and THERMOCALC and were found to be identical to within 0.1 °C in all cases. Reactions involving fluids may differ somewhat, because of the different equations of state used e.g. for H2O in the various programs. Formula units computed with CalcFormula have been checked against results of the programs HYPER-FORM (Bjerg et al., 1992) and EMP-AMPH (Mogessie and others, 1990), ideal mixing on site activities against the output of RECALC.EXE, available with the THERMOCALC software. Forthcoming updates of PET will also include the thermodynamic data set of Gottschalk (1996), as well as functions for plotting mineralchemical data (triangle and xy-plots).

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Appendix: List of PET files and their contents (all ASCII format)

PET files that contain Mathematica programs

FILENAME	contains the PET functions
ABT.M	Agt
ACPX.M	Acpx
AFS.M	Afs
AGT.M	Agt
AMS.M	Ams
DEFDAT.M	DatasetType, PET
DGH2H2O.M	Dgr, ConvertXh2, CalcRea
DGO2.M	Dgr, CalcRea
DGPT.M	Dgr, CalcRea
DGXC.M	Dgr, CalcRea
FORMEL.M	CalcFormula, ExtractSampleDat, MakeAnalysisTable, TransformDatFile
G.M	MinDat, MinList, GOrdAb, GOrd, G
GTB.M	CalcThermoBaro plus all geothermobarometer functions

H2OCO2KJ.M Vh2o, Fkh2o, Fh2o, Vco2, Fkco2, Fco2, Vh2oco2, Fkh2om, Ah2o, Fkco2m, Aco2

H2OH2.M CalcVol, Vh2oh2, FFkh2o, FFkh2, FFkh2om, FFkh2m, AAh2o, AAh2

UTILITY.M O2buffers, ConvertLogfo2, SaveRea, GetRea, PlotRea, MakeRea, MakeAllRea, SelectRea, SelectIncompRea, CalcReaIntersection, InsertPhase, DeletePhase, ProjectionSymbolic, Projection

Data files

CHEM.M chemical data file

THDATB.M thermodynamic data file (Berman data set)

THDATHP.M thermodynamic data file (Holland and Powell data set)

Auxiliary data files

GTB mineralchemical data of 16 minerals in order to test CalcThermoBaro

HS78B mineralchemical data example file (sample 78B of Hodges and Spear, 1982) HS78B.EMP microprobe data file (structure as created by a JEOL-JX 8600 microprobe) convertable by TransformDatFile to

HS78B README.TXT PET installation and documentation file

Mathematica example file

EXAMPLES contains 39 examples of the usage of PET functions