

ECBAR96 description and instructions

ECBAR is a stand-alone program for calculating pressures and temperatures using the garnet-clinopyroxene-phengite geobarometer (Waters and Martin, 1993) in conjunction with the garnet-clinopyroxene geothermometer. It employs a Monte-Carlo error-propagation technique to estimate the uncertainty on the P-T estimate and to investigate the contribution of each mineral end member activity term to the overall result.

The current version, `ecbar96.exe`, uses code dating from March 1996, and has been recompiled for modern Windows systems, where it runs in a command prompt window. ECBAR uses the calibration described at <http://www.earth.ox.ac.uk/~davewa/research/eclogites/ecbarcal.html> including the empirical adjustment that minimises the discrepancy between calculated and experimental pressures in the study by Schmidt (1993). The thermometer calibration is that of Powell (1985).

References

- Waters DJ, Martin HN (1993) Geobarometry in phengite-bearing eclogites. *Terra Abstracts* 5 (1): 410-411.
- Powell, R (1985) Regression diagnostics and robust regression in geothermometer/geobarometer calibration; the garnet-clinopyroxene geothermometer revisited. *Journal of Metamorphic Geology*. 3, 231-243.
- Schmidt, MW (1993) Phase relations and compositions in tonalite as a function of pressure; an experimental study at 650°C. *American Journal of Science*, 293, 1011-1060.

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What ECBAR does

The program accepts mineral analyses of garnet, clinopyroxene and phengite in weight percent oxides, either interactively or from a text file. Data entered interactively can be saved in a format which can subsequently be read as an input file, or used as a template for further input files.

ECBAR now asks for information about this run of the program: an estimated temperature of equilibration (which can be adjusted at the next step), a choice of garnet and pyroxene activity models, and a parameter to control the overall uncertainty on the mineral analyses.

ECBAR now recalculates the mineral analyses into cations per formula unit, and applies the garnet-clinopyroxene geothermometer. You now have the choice of adopting a suitable fixed temperature, or of allowing ECBAR to calculate both pressure and temperature.

Whatever your choice, the program now calculates pressures using the input mineral data, at the T of interest, and also at T+50 and T-50 degrees, to indicate the slope of the barometer equilibrium.

Next comes the Monte-Carlo error propagation. Basically, the pressure calculation is now repeated a large number of times, while at each step the input weight percentages for all three minerals are varied by choosing values at random from an appropriately-scaled gaussian distribution around the measured value for each oxide. Currently there are 200 steps. The program outputs the mean of the calculated pressures (and temperatures, if these too were allowed to vary), together with the calculated standard deviation and other statistical parameters. The Monte-Carlo propagation is done twice, once including uncertainties on weight percents only, and then again with the further inclusion of uncertainties on the

mixing parameters for activity models (these are held internally in the program, the values being taken from the source references). The contribution of each end member to InK is shown separately, so that you can assess the sensitivity of your input data.

The program creates two output files, one called `ecbar.res`, which contains the summary of results you see on the screen, and another called `ecbarpt.res`, which is a simple list of the temperatures and pressures generated at each of the Monte-Carlo cycles. This latter file could be used to get a visual display of the error cloud, or processed for further estimation of the P-T error ellipse.

How to run ECBAR

This is a text-based program with a simple command-line interface. Yes, I know this is an old-fashioned way to do things, but the original program dates from 1991, and I am unlikely in the near future to produce a Windows GUI version.

Under Windows the program runs in a command prompt box, and can be started using the run command on the Start Menu or by double-clicking the executable file in Windows File Explorer.

The program requires two types of response from the user:

- Questions with yes/no answers, to which you type `y` or `n` (upper or lower case). If the desired answer is yes, a simple carriage return is sufficient.
- Numerical or text input. The quality of the error-trapping is variable - you may get uninformative error-messages if you enter something unexpected!

Step by step

Answer **yes** (y or 'Enter') to the first question

```
Output to file (ECBAR.RES)? (y) :
```

as any other response causes an immediate crash (under DOS you could direct output straight to the printer).

Next, answering **no** to

```
Data from a file? (y) :
```

takes you to the interactive input of data.

It is recommended that you enter your first sample interactively, then save the input data to one of the text file formats for use as a template. In detail the file formats are intended to harmonise with my own personal mineral database format (Lotus 123, circa 1988!), but with a little care you could set up an Excel worksheet to generate data files in the correct format.

If input is from a file, you are asked to supply the file name (and path, if needed).

The program checks it can read the file properly - it should report that it has found the expected oxides in the correct order - before asking you if it is OK to continue.

```
Checking that oxides are in correct sequence ...
Expected:  SiO2 TiO2 Al2O3 Fe2O3 FeO MnO MgO CaO Na2O K2O
File has:  SiO2 TiO2 Al2O3 Fe2O3 FeO MnO MgO CaO Na2O K2O
Do you want to continue? (y) :
```

Now you must supply a "seed" temperature for the calculation (for the first cycle of activity calculation), and select activity models for garnet and pyroxene.

Temperature (C) :

Choose garnet mixing model:

- 1 = Ganguly & Saxena 1984 without ternary approx
- 2 = Geiger et al 87, Fe-Mg-Ca mixing
- 3 = Simple Mg-Ca mixing, Newton & Haselton 1981
- 4 = Mg-Ca (NH81) + Fe-Mg after Hackler & Wood 89
- 5 = Ideal quaternary mixing
- 6 = Berman 1990 Am Min 75
- 7 = Sengupta et al 1989 (CMP) extension of GS-84

choice :

Disordered (two-site) Cpx? (y) :

For consistency with the calibration, the simple Mg-Ca mixing model of Newton and Haselton should be used for absolute P determination. You are welcome to examine how sensitive the result is to a different choice of activity model! In general, a higher pressure may result from the more complex mixing models. For pyroxene there is a choice between the non-ideal 2-site model of Holland (1990, CMP 105: 446-53) for Na-bearing C2/c pyroxenes, or a simple 1-site model for ordered omphacite. Before deciding which to use for lower-T eclogites, it might be worth reflecting on whether you believe the pyroxene grew, and approached equilibrium, in a disordered or an ordered state, given that most such pyroxenes show antiphase domain microstructures.

Analytical uncertainty (as % error on 100%; try 1) : 1

The analytical uncertainty applied by ECBAR assumed that the error is random and dominated by X-ray counting statistics. You input an estimate of the 2sigma on an element present at a concentration of 100%, and these are then scaled so that the absolute error on any element is proportional to the square root of the actual weight percent. For well-behaved wavelength spectrometers the appropriate value is about 1; for EDS systems make it a bit bigger.

Now you get some mineral recalculation output, and a calculated temperature, e.g.

	SiO2	TiO2	Al2O3	Fe2O3	FeO	MnO	MgO	CaO	Na2O	K2O	Total
Garnet	40.20	0.00	23.20	0.62	16.84	0.18	11.90	7.68	0.00	0.00	100.62
	2.972	0.000	2.022	0.034	1.041	0.011	1.311	0.608	0.000	0.000	8.000
Clinopx	55.40	0.09	9.09	0.01	2.11	0.03	11.30	17.10	4.76	0.00	99.89
	1.972	0.002	0.381	0.000	0.063	0.001	0.599	0.652	0.328	0.000	3.999
Phengite	51.40	0.40	26.90	0.95	0.23	0.00	4.08	0.04	1.15	9.82	94.97
	3.411	0.020	2.105	0.047	0.013	0.000	0.404	0.003	0.148	0.831	6.982

Estimated T (Powell 1985) is 710 (C)

Keep T fixed at trial value? (y) :

Answering **no** here gives you the opportunity to examine the uncertainty on calculated temperature as well as pressure:

Use variable Powell 1985 temperatures? (y) :

and a further **no** here allows you to supply any other fixed temperature value.

Now (after showing you the matrix of garnet interaction parameters) the program begins to give you some results based on the mineral data exactly as input,, which allow you to plot a section of the P-T

curve for the barometer equilibrium. The calculated activities are listed; the $\ln a(\text{Mica})$ term is $\ln a(\mu) - \ln a(\text{cel})$.

T (C)	P (kbar)	$\ln a(\text{prp})$	$\ln a(\text{grs})$	$\ln a(\text{di})$	$\ln a(\text{Mica})$	$\ln K$
648	22.64	-2.1246	-3.6919	-0.5703	0.4490	7.4338
698	22.00	-2.1563	-3.7889	-0.5907	0.4490	7.5370
748	21.35	-2.1850	-3.8764	-0.6091	0.4490	7.6302

Finally, you have the option (highly recommended) to do the Monte-Carlo error propagation:

Do Monte-Carlo error propagation? (y) :

... and two blocks of results, based on random perturbations of the input mineral analyses, are generated. The second block includes uncertainty on the interaction parameters used in the activity models for garnet and clinopyroxene. The moment statistics are listed for each set of results. If temperatures are allowed to vary, an uncertainty is also given for the thermometer calculation.

Results of Monte-Carlo error propagation: weight % only

	Mean	s.d.	skew	kurt
T (C)	695	20	-0.205	-0.025
P (kbar)	22.053	1.275	0.457	1.103
$-\ln(\text{Prp})$	2.159	0.075	0.045	-0.192
$-2\ln(\text{Grs})$	7.580	0.202	-0.051	-0.088
$6\ln(\text{Di})$	-3.545	0.191	-0.044	-0.158
$3\ln(\text{Mica})$	1.334	0.250	0.033	-0.550
$\ln K$	7.528	0.380	-0.421	1.024

Results of Monte-Carlo error propagation: wt% and mixing params

	Mean	s.d.	skew	kurt
T (C)	696	20	-0.011	-0.451
P (kbar)	21.815	1.440	0.222	-0.276
$-\ln(\text{Prp})$	2.165	0.076	-0.060	-0.244
$-2\ln(\text{Grs})$	7.591	0.200	0.026	-0.361
$6\ln(\text{Di})$	-3.530	0.289	-0.101	-0.333
$3\ln(\text{Mica})$	1.369	0.248	0.116	-0.085
$\ln K$	7.595	0.423	-0.229	-0.277

Keep a look-out for asymmetrical results (best seen in the skewness column) or other abnormal behaviour. The mineral formula recalculation can be rather non-linear, particularly for clinopyroxenes when Fe^{3+} recalculation is being done. See below under tricks and tips for advice.

Tricks & tips

Fe^{3+} is not recalculated if there is already an entry for Fe_2O_3 . You can prevent ferric iron recalculation by assigning a finite but negligible value, such as 0.001%, to Fe_2O_3 . Commonly, this will cure the non-linear behaviour of some pyroxenes during the Monte-Carlo error propagation.