

## Web-Based (PYTHON) Version of RCLC:

**Reference to be Cited:** Pattison, D.R.M, Chacko, T., Farquhar, J. & McFarlane, C.R.M. (2003) Temperatures of granulite-facies metamorphism: constraints from experimental phase equilibria and thermobarometry corrected for retrograde exchange. *Journal of Petrology*, 44, 867-900.

### Overview of the RCLC Program

**RCLC**, which is short for ‘recalculation’, is a program that calculates pressure-temperature (P-T) conditions of Grt-Opx-Pl-Qtz±Crd±Bt assemblages based on Al-solubility in Opx in equilibrium with Grt, corrected for late Fe-Mg exchange.

The rationale and calculation method for the program are described in Chacko et al. (1996) and in Pattison et al. (2003). Fig. 3 of Pattison et al. (2003) shows graphically how **RCLC** works.

The program described in Pattison et al. (2003) was written in BASIC and compiled on a PC. However, because the BASIC language is no longer compatible with newer versions of the Windows operating system, the **RCLC** program was converted into a Web-based application in which the underlying computer code is written in the PYTHON programming language.

**RCLC** was originally written by Tom Chacko and James Farquhar in 1996 and subsequently modified by Chris McFarlane, David Pattison and Tom Chacko between 1997 and 2002. The Web-based version of **RCLC** was developed by Justin Widney of the University of Alberta in 2018 as part of an undergraduate summer internship.

### Input Data for RCLC

**RCLC** requires the following input for the calculation of P-T in a sample: mineral composition and modal abundance data for garnet and orthopyroxene and mineral composition data for plagioclase. Although not required for the calculation, if present, the modes and compositions of biotite and/or cordierite can also be included in the calculations to correct for retrograde Fe-Mg exchange between those phases and garnet and orthopyroxene in the rock. The compositional data for all of these minerals must be recalculated off-line by the user into atomic proportions of cations on the following basis: Grt (12 oxygens), Opx (6 oxygens or 4 cations), Crd (18 oxygens), Bt (11 oxygens) and Pl (8 oxygens). The cation proportion data for each mineral and the modal abundance data for Grt, Opx, ± Bt, ± Crd are typed into the appropriate cell in the mineral composition/modal abundance input table on the webpage. The user must also select one or more Al-in-opx models for calculating the proportion of the octahedral site in opx filled by Al (see below).

Two example inputs are shown below. **PCFM-1** is the sample in Table 4 and Fig. 3 of Pattison et al. (2003). (Note that there is a slight difference in the example shown below compared to Fig. 3 of Pattison et al. (2003), because the modes of Crd and Bt have been set to 10.0 and 10.0, respectively, rather than 0.0 and 0.0 as in Fig. 3). Sample **165-241** is from Chacko et al. (1987; 1996). If there is no Crd or Bt in the rock, as in **165-241**, zeroes are inserted and the program still works. Only one Al-in-opx model was chosen for **PCFM-1** (Model 2) whereas all four Al-in-opx models were chosen for **165-241**.

## PCFM-1

PCFM-1

GARNET				
Fe	Mn	Mg	Ca	MODEGAR
1.550	0.200	1.140	0.110	10.0

ORTHOPIYOXEN									
Si	Ti	Al	Cr	Fe3	Fe2	Mn	Mg	Ca	MODEOPX
1.900	0.010	0.200	0.000	0.000	0.660	0.010	1.230	0.000	10.0

CORDIERITE			
Fe	Mn	Mg	MODECRD
0.340	0.010	1.660	10.0

BIOTITE								
Si	Ti	Al	Fe	Mn	Mg	Na	K	MODEBT
2.760	0.240	1.300	0.780	0.010	1.780	0.010	0.970	10.0

PLAGIOCLASE		
Ca	Na	K
0.310	0.670	0.020

## Al-in-opx MODEL

- 1: XALM = Al - ( 2 - Si)  
 2: XALM = Al/2  
 3: XALM = (Al/2) / (Fe2+ + Mg + Mn + Ca + (Al/2) )  
 4: XALM = (AL- Fe3+ - Cr - (2\*Ti) ) / 2

Submit

## 165-241

165-241

GARNET				
Fe	Mn	Mg	Ca	MODEGAR
1.842	0.175	0.849	0.191	10.0

ORTHOPIYOXEN									
Si	Ti	Al	Cr	Fe3	Fe2	Mn	Mg	Ca	MODEOPX
1.864	0.003	0.227	0.000	0.037	0.851	0.029	0.969	0.015	40.0

CORDIERITE			
Fe	Mn	Mg	MODECRD
0.000	0.000	0.000	0.0

BIOTITE								
Si	Ti	Al	Fe	Mn	Mg	Na	K	MODEBT
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0

PLAGIOCLASE		
Ca	Na	K
0.354	0.581	0.045

## Al-in-opx MODEL

- 1: XALM = Al - ( 2 - Si)  
 2: XALM = Al/2  
 3: XALM = (Al/2) / (Fe2+ + Mg + Mn + Ca + (Al/2) )  
 4: XALM = (AL- Fe3+ - Cr - (2\*Ti) ) / 2

Submit

### Fe<sup>3+</sup> and minor elements in Opx

As shown above, **RCLC** allows Fe<sup>3+</sup> and Fe<sup>2+</sup> in Opx to be entered separately. The Fe<sup>2+</sup>/Fe<sup>3+</sup> calculation is done beforehand by the user (it is not performed in **RCLC**). If all Fe is assumed to be Fe<sup>2+</sup> (such as in **PCFM-1**), zero is inserted for Fe<sup>3+</sup>.

### Al-in-Opx Models

The Al-in-opx model calculates the proportion of the octahedral site of Opx filled by Al (**XALM**). Four models are available for making this calculation:

- 1: **XALM** = **Al** - (2 - **Si**)
- 2: **XALM** = **Al**/2
- 3: **XALM** = (**Al**/2) / (**Fe**2+ + **Mg** + **Mn** + **Ca** + (**Al**/2) )
- 4: **XALM** = (**Al** - **Fe**3+ - **Cr** - (2\***Ti**) ) / 2

The pros and cons of the different models are discussed in Pattison et al. (2003). In that paper, we used Model 2 because it allowed comparison between a large number of samples from the literature, some of which reported minor elements and Fe<sup>3+</sup> and others which did not. Model 4 is the only model that allows a correction for Fe<sup>3+</sup> in Opx, although there can be dangers in taking this approach because of imprecision in schemes for estimating Fe<sup>3+</sup> in Opx from stoichiometry (see discussion in Pattison et al., 2003).

The program does the Al-in-opx calculations and allows the user to compare the effects of the different models on the resulting P and T.

### Running the RCLC Program

Once the mineral composition and modal abundance data for the sample have been typed into input table and one or more Al-in-Opx models have been selected, click the SUBMIT button to run the P-T calculations.

The results of the calculations are outputted in table form on the webpage and also as an Excel CSV file that can be downloaded (click button for download)

## Program Outputs

### Example #1 of output from RCLC - PCFM-1

The Excel csv file outputs from RCLC for PCFM-1 and 165-241 are shown below. PCFM-1 will be used to describe the parameters listed in the output. Only Model 2 for  $X_{Al}^{Opx}$  was chosen for this run.

PCFM-1

TITLE = MODEL 2  $X_{Al}^{Opx}$  (1-site Opx) = (Al/2) / 2XFeOpx = Fe<sup>2+</sup>/2 XMgOpx = Mg/2

ModeGrt= 10 ModeOpx= 10 ModeBt= 10 ModeCrd= 10  
 XFeGrt= 0.517 XMgGrt= 0.38 XMnGrt= 0.067 XcaGrt= 0.037  
 XFeOpx= 0.33 XMgOpx= 0.615 XAlOpx= 0.05 TotOpx= 1.005  
 XFeBt= 0.272 XMgBt= 0.62 XAlBt= 0.021 XTiBt= 0.084  
 XFeCrd= 0.169 XMgCrd= 0.826 XMnCRD = 0.005  
 XAnPl= 0.31 XAbPl= 0.67

INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS

	CONVERGED(FINAL)		INITIAL		DIFFERENCE	
Fe Al GOPQ	857 C	7.76 KB	808C	7.63KB	50C	0.13 KB
GrtOpx GOPQ	857 C	7.76 KB	704 C	6.28 KB	154C	1.48 KB
GrtBt GOPQ	857 C	7.76 KB	667 C	5.81 KB	191C	1.95 KB
GrtCrd GOPQ	857 C	7.76 KB	695 C	6.16 KB	163C	1.59 KB
M/FM rock	0.613		0.613		0	
M/FM Grt	0.472		0.424		0.048	
M/FM Opx	0.647		0.651		-0.004	
M/FM Bt	0.661		0.695		-0.035	
M/FM Crd	0.781		0.83		-0.049	

### Explanation of RCLC output

Following the sample number and sample description, the chosen  $X_{Al}^{Opx}$  model is specified and the Opx compositional parameters further down are defined. The modes and some key mineral compositional parameters as inputted by the user are then listed. Definitions of some of the compositional parameters are as follows:

$$xiGrt = i/(Fe+Mg+Ca+Mn)$$

$$TotOpx = X_{Al}^{Opx} + FeOpx + XMgOpx + Ti/2 + Fe^{3+}/2 + Cr/2 + Mn/2 + Ca/2^*$$

$$xiBt = i/(Fe+Mg+Mn+Ti+Al^{vi}) \text{ where } Al^{vi} = Al^{tot} - (4 - Si)$$

$$xiCrd = i/(Fe+Mg+Mn)$$

$$xiPl = i/(Ca+Na+K)$$

\* Note that regardless of choice of  $X_{Al}^{Opx}$  model, TotOpx (total octahedral cations for a one-site Opx) includes all minor elements.\*

The initial and converged P-T estimates and Mg/(Mg+Fe) ratios are then listed, along with the differences between those two sets of estimates. The quantities are defined as follows:

**Fe Al GOPQ** = intersection of equilibria 8 (Fe-end member Grt-Opx Al-solubility equilibrium) and 9 (Fe-end member Grt-Opx-Pl-Qtz equilibrium). The 'initial' values are for the Fe-Mg ratios of the measured minerals and correspond to point B in Fig. 3a of Pattison et al. (2003), whereas the 'converged' values correspond to point C in Fig. 3b.

**GrtOpx GOPQ** = intersection of equilibria 7 (Grt-Opx Fe-Mg exchange equilibrium) and 9 (Fe-end member Grt-Opx-Pl-Qtz equilibrium). The 'initial' values are for the Fe-Mg ratios of the measured minerals and correspond to point A in Fig. 3a of Pattison et al. (2003), whereas the 'converged' values correspond to point C in Fig. 3b.

**GrtBt GOPQ** = intersection of Grt-Bt Fe-Mg exchange equilibrium with equilibrium 9 (Fe-end member Grt-Opx-Pl-Qtz equilibrium). The 'initial' values are for the Fe-Mg ratios of the measured minerals, whereas the 'converged' values are for point C in Fig. 3b.

**GrtCrd GOPQ** = intersection of Grt-Crd Fe-Mg exchange equilibrium with equilibrium 9 (Fe-end member Grt-Opx-Pl-Qtz equilibrium). The 'initial' values are for the Fe-Mg ratios of the measured minerals, whereas the 'converged' values are for point C in Fig. 3b.

**M/FM rock** = Mg/(Mg+Fe) of whole rock based on modes of Grt, Opx, Crd and Bt and their Mg/(Mg+Fe) ratios. After varying the Mg/(Mg+Fe) ratios of the phases to obtain convergence at point C in Fig. 3b, the whole rock Mg/(Mg+Fe) is recalculated to ensure that it is the same as the initial value.

**M/FM Grt** = Mg/(Mg+Fe) of Grt.

**M/FM Opx** = Mg/(Mg+Fe) of Opx.

**M/FM Bt** = Mg/(Mg+Fe) of Bt.

**M/FM Crd** = Mg/(Mg+Fe) of Crd.

\*\* Remember that the calculated values above are slightly different than those shown in Fig. 3 of Pattison et al. (2003) because the mineral modes are different. \*\*

## Example #2 of output from RCLC - 165-241

The output for 165-241 is listed below and shows the effect of using different  $X_{Al}^{Opx}$  models. The  $Fe^{3+}$ -corrected  $X_{Al}^{Opx}$  model (Model 4) gives lower temperatures by about 50 °C than the simple Al/2 model (Model 2).

165-241

TITLE = MODEL 1  $X_{Al}^{Opx}$  (1-site Opx) =  $(Al - (2 \cdot Si)) / (2X_{Fe}^{Opx} + Fe_2 + 2)$   $X_{Mg}^{Opx} = Mg/2$

ModeGrt=	10	ModeOpx=	40	ModeBt=	0	ModeCr=	0
XFeGrt=	0.603	XMgGrt=	0.278	XMnGrt=	0.057	XcaGrt=	0.062
XFeOpx=	0.425	XMgOpx=	0.484	XAlOpx=	0.046	TotOpx=	0.997
XFeBt=	0	XMgBt=	0	XAlBt=	0	XTiBt=	0
XFeCr=	0	XMgCr=	0	XMnCr=	0		
XAnPl=	0.361	XAbPl=	0.593				

INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS

		CONVERGED(FINAL)		INITIAL		DIFFERENCE	
Fe Al	GOPQ	944 C	8.88 KB	905C	8.74KB	39C	0.14 KB
GrtOpx	GOPQ	944 C	8.88 KB	793 C	7.14 KB	151C	1.74 KB
GrtBt	GOPQ	0 C	8.88 KB	0 C	0.00 KB	0C	8.88 KB
GrtCr	GOPQ	0 C	8.88 KB	0 C	0.00 KB	0C	8.88 KB
M/FM	rock	0.495		0.495			0
M/FM	Grt	0.352		0.315			0.037
M/FM	Opx	0.525		0.532			-0.008
M/FM	Bt	0		0			0
M/FM	Cr	0		0			0

TITLE = MODEL 2  $X_{Al}^{Opx}$  (1-site Opx) =  $(Al/2) / (2X_{Fe}^{Opx} + Fe_2 + 2)$   $X_{Mg}^{Opx} = Mg/2$

ModeGrt=	10	ModeOpx=	40	ModeBt=	0	ModeCr=	0
XFeGrt=	0.603	XMgGrt=	0.278	XMnGrt=	0.057	XcaGrt=	0.062
XFeOpx=	0.425	XMgOpx=	0.484	XAlOpx=	0.057	TotOpx=	1.009
XFeBt=	0	XMgBt=	0	XAlBt=	0	XTiBt=	0
XFeCr=	0	XMgCr=	0	XMnCr=	0		
XAnPl=	0.361	XAbPl=	0.593				

INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS

		CONVERGED(FINAL)		INITIAL		DIFFERENCE	
Fe Al	GOPQ	1026 C	9.89 KB	963C	9.65KB	63C	0.24 KB
GrtOpx	GOPQ	1026 C	9.89 KB	788 C	7.13 KB	238C	2.76 KB
GrtBt	GOPQ	0 C	9.89 KB	0 C	0.00 KB	0C	9.89 KB
GrtCr	GOPQ	0 C	9.89 KB	0 C	0.00 KB	0C	9.89 KB
M/FM	rock	0.495		0.495			0
M/FM	Grt	0.37		0.315			0.054
M/FM	Opx	0.521		0.532			-0.011
M/FM	Bt	0		0			0
M/FM	Cr	0		0			0

TITLE = MODEL 3  $X_{Al}^{Opx}$  (1-site Opx) =  $(Al/2) / (\text{sum where sum} = Fe_2 + Mg + Mn + Ca + (Al/2))$ .  $X_{Fe}^{Opx} = Fe_2 / \text{sum}$

ModeGrt=	10	ModeOpx=	40	ModeBt=	0	ModeCr=	0
XFeGrt=	0.603	XMgGrt=	0.278	XMnGrt=	0.057	XcaGrt=	0.062
XFeOpx=	0.43	XMgOpx=	0.49	XAlOpx=	0.057	TotOpx=	1.02
XFeBt=	0	XMgBt=	0	XAlBt=	0	XTiBt=	0
XFeCr=	0	XMgCr=	0	XMnCr=	0		
XAnPl=	0.361	XAbPl=	0.593				

INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS

		CONVERGED(FINAL)		INITIAL		DIFFERENCE	
Fe Al	GOPQ	1030 C	9.95 KB	965C	9.56KB	66C	0.38 KB
GrtOpx	GOPQ	1030 C	9.95 KB	787 C	7.02 KB	244C	2.93 KB
GrtBt	GOPQ	0 C	9.95 KB	0 C	0.00 KB	0C	9.95 KB
GrtCr	GOPQ	0 C	9.95 KB	0 C	0.00 KB	0C	9.95 KB
M/FM	rock	0.495		0.495			0
M/FM	Grt	0.371		0.315			0.055
M/FM	Opx	0.521		0.532			-0.011
M/FM	Bt	0		0			0
M/FM	Cr	0		0			0

TITLE = MODEL 4  $X_{Al}^{Opx}$  (1-site Opx) =  $((Al - Fe_3 + - Cr - (2 \cdot Ti)) / 2) / (2X_{Fe}^{Opx} + Fe_2 + 2)$   $X_{Mg}^{Opx} = MgOpx/2$

ModeGrt=	10	ModeOpx=	40	ModeBt=	0	ModeCr=	0
XFeGrt=	0.603	XMgGrt=	0.278	XMnGrt=	0.057	XcaGrt=	0.062
XFeOpx=	0.425	XMgOpx=	0.484	XAlOpx=	0.046	TotOpx=	0.998
XFeBt=	0	XMgBt=	0	XAlBt=	0	XTiBt=	0
XFeCr=	0	XMgCr=	0	XMnCr=	0		
XAnPl=	0.361	XAbPl=	0.593				

INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS

		CONVERGED(FINAL)		INITIAL		DIFFERENCE	
Fe Al	GOPQ	948 C	8.92 KB	908C	8.78KB	40C	0.15 KB
GrtOpx	GOPQ	948 C	8.92 KB	793 C	7.14 KB	155C	1.78 KB
GrtBt	GOPQ	0 C	8.92 KB	0 C	0.00 KB	0C	8.92 KB
GrtCr	GOPQ	0 C	8.92 KB	0 C	0.00 KB	0C	8.92 KB
M/FM	rock	0.495		0.495			0
M/FM	Grt	0.353		0.315			0.037
M/FM	Opx	0.525		0.532			-0.008
M/FM	Bt	0		0			0
M/FM	Cr	0		0			0