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 Webbased 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, \pm Bt, \pm 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		<u>In</u>	Mg	;	Ca		MODEG	AR						
1.550	0.200		1.140		0.110		10.0							
ORTHOPY	ROXE	EN												
Si			Ti		Al		Cr		Fe3	Fe2	Mn	Mg	Ca	
1.900		0.01	0	0.20	0	0.00	0	0.00	0	0.660	0.010	1.230	0.000	10.0
CORDIERI	TE													
Fe		Mn		Mg	MO	DEC	RD							
0.340	0.0	010	1.66	0	10.0									
BIOTITE														
Si]	Гi	Al		Fe		Mn		Mg	Na	K	MODE	BT	
2.760	0.240		1.300		0.780		0.010		1.780	0.010	0.970	10.0		
PLAGIOCI	LASE													
Ca		Na	a	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	М	Ín	M	2	Ca		MODEG	AR								
1.842	0.175		0.849		0.191		10.0									
ORTHOPY	ROXE	N														
Si			Ti		Al		Cr		Fe3	Fe2		/In	Mg	(Ca	MODEOPX
1.864		0.00)3	0.22	27	0.00	0	0.03	7	0.851	0.029		0.969	0.015		40.0
CORDIERI	ITE															
Fe		Mn		Mg	MO	DEC	RD									
0.000	0.0	00	0.00	0	0.0											
BIOTITE																
Si	Т	ï	A		Fe		Mn		Mg	Na		K	MODE	BT		
0.000	0.000		0.000		0.000		0.000		0.000	0.000	0.	.000	0.0			
PLAGIOCI	LASE															
Ca		Na	a	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

Fe³⁺ and minor elements in Opx

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

Al-in-Opx Models

The Al-in-opx model calculates the proportion of the octahedal 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) / (Fe2+ + Mg + Mn + Ca + (Al/2) )

4: XALM = (Al - Fe3+ - 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^{3+} and others which did not. Model 4 is the only model that allows a correction for Fe^{3+} in Opx, although there can be dangers in taking this approach because of imprecision in schemes for estimating Fe^{3+} in Opx from stoichiometry (see discussion in Pattison et al., 2003).

The program does the Al-in-opx calculations and 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

MODEL 2 XAIOpx (1-site Opx) = (AI/2) / 2XFeOpx = Fe2+/2 XMgOpx = Mg/2 TITLE =

ModeGrt= XFeGrt= XFeOpx= XFeBT=		XMgGrt= XMgOpx= XMgBt=	0.38 0.615 0.62	ModeBt= XMnGrt= XAlOpx= XAlBt=	0.05 0.021	XcaGrt= TotOpx=	10 0.037 1.005 0.084			
XFeCrd=		XMgCrd=		XMnCRD =	0.005					
XAnPl=	0.31	XAbPI=	0.67							
INITIAL AND CC	-	T ESTIMATES AI RGED(FINAL)	ND MINER	AL COMPOSI	TIONS 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	3		0			
M/FM Grt 0.472				0.424	ļ	0.048				
M/FM Opx				0.652	L	-0.004				
M/FM Bt	0.661			0.695	5	-0.035				
M/FM Crd	0.781			0.83	3		-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) $TotOpx = XAlopx + FeOpx + XMgOpx + Ti/2 + Fe^{3+}/2 + Cr/2 + Mn/2 + Ca/2*$ **xibt** = $i/(Fe+Mg+Mn+Ti+Al^{vi})$ 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.

GFEBE 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 Fe³⁺-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 XA	lOpx (1-site Op	ox) = (Al - (2	-Si))/2XFeO	px = Fe2+/2	XMgOpx = N	1g/2		
ModeGrt=	10	ModeOpx=	40	ModeBt=	0	ModeCrd=		0	
XFeGrt=	0.603	XMgGrt=	0.278	XMnGrt=	0.057	XcaGrt=		0.062	
XFeOpx=	0.425	XMgOpx=	0.484	XAIOpx=	0.046	TotOpx=		0.997	
XFeBT=		XMgBt=		XAIBt=		XTiBt=		0	
XFeCrd=		XMgCrd=		XMnCRD =	0				
XAnPI=		XAbPI=	0.593						
INITIAL AND CO		RGED(FINAL)	ND WIINER/	AL COMPOSIT	INITIAL				DIFFERENCE
Fe Al GOPQ	944 C	8.88 KB		905C	8.74KB		39C		0.14 KB
GrtOpx GOPQ		8.88 KB		793 C	7.14 KB		1510		1.74 KB
GrtBt GOPQ	0 C	8.88 KB		0 C	0.00 KB		0C		8.88 KB
GrtCrd GOPQ M/FM rock	0 C 0.495	8.88 KB		0 C 0.495	0.00 KB		0C	0	8.88 KB
M/FM Grt	0.495			0.495				0.037	
M/FM Opx	0.525			0.532				-0.008	
M/FM Bt	0			C				0	
M/FM Crd	0			C				0	
TITLE =	MODEL 2 XA	lOpx (1-site Op	ox) = (AI/2)	/ 2XFeOpx =	Fe2+/2 XMg	Opx = Mg/2			
ModeGrt=		ModeOpx=		ModeBt=		ModeCrd=		0	
XFeGrt=		XMgGrt=		XMnGrt=		XcaGrt=		0.062	
XFeOpx=		XMgOpx=		XAIOpx=		TotOpx=		1.009	
XFeBT=		XMgBt=	0	XAIBt=		XTiBt=		0	
XFeCrd=		XMgCrd=		XMnCRD =	0				
XAnPI=		XAbPI=	0.593						
INITIAL AND CO		T ESTIMATES A RGED(FINAL)	ND MINERA	AL COMPOSIT	IONS				DIFFERENCE
Fe Al GOPQ	1026 C	9.89 KB		963C	9.65KB		63C		0.24 KB
GrtOpx GOPQ		9.89 KB		788 C	7.13 KB		2380		2.76 KB
GrtBt GOPQ	0 C	9.89 KB		0 C	0.00 KB		0C		9.89 KB
GrtCrd 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 M/FM Opx	0.37 0.521			0.315				0.054	
M/FM Bt	0.521								
				0					
M/FM Crd	0			C				0 0	
M/FM Crd TITLE = ModeGrt=	MODEL 3 XA	lOpx (1-site Op ModeOpx=		C	sum = Fe2+ + 0	ModeCrd=	a + (Al	0	eOpx = Fe2+/sum
TITLE = ModeGrt= XFeGrt=	MODEL 3 XA 10 0.603	ModeOpx= XMgGrt=	40 0.278	0 / sumwhere ModeBt= XMnGrt=	sum = Fe2+ + 0 0.057	ModeCrd= XcaGrt=	a + (Al	0 /2). XFe 0 0.062	20px = Fe2+/sum
TITLE = ModeGrt= XFeGrt= XFeOpx=	MODEL 3 XA 10 0.603 0.43	ModeOpx= XMgGrt= XMgOpx=	40 0.278 0.49	0 / sumwhere ModeBt= XMnGrt= XAIOpx=	sum = Fe2+ + 0 0.057 0.057	ModeCrd= XcaGrt= TotOpx=	a + (Al	0 /2). XFe 0 0.062 1.02	20px = Fe2+/sum
TITLE = ModeGrt= XFeGrt= XFeOpx= XFeBT=	MODEL 3 XA 10 0.603 0.43 0	ModeOpx= XMgGrt= XMgOpx= XMgBt=	40 0.278 0.49 0	/ sumwhere ModeBt= XMnGrt= XAIOpx= XAIBt=	sum = Fe2+ + 0 0.057 0.057 0	ModeCrd= XcaGrt=	a + (Al	0 /2). XFe 0 0.062	20px = Fe2+/sum
TITLE = ModeGrt= XFeGrt= XFeOpx=	MODEL 3 XA 10 0.603 0.43 0 0	ModeOpx= XMgGrt= XMgOpx=	40 0.278 0.49 0	o / sumwhere ModeBt= XMnGrt= XAIOpx= XAIBt= XMnCRD =	sum = Fe2+ + 0 0.057 0.057	ModeCrd= XcaGrt= TotOpx=	ia + (Al	0 /2). XFe 0 0.062 1.02	2Opx = Fe2+/sum
TITLE = ModeGrt= XFeGrt= XFe0px= XFeBT= XFeCrd=	MODEL 3 XA 10 0.603 0.43 0 0.361 DNVERGED P-	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A	40 0.278 0.49 0 0 0.593	/ sumwhere ModeBt= XMnGrt= XAIOpx= XAIBt= XMnCRD =	sum = Fe2+ + 0 0.057 0.057 0 0 710NS	ModeCrd= XcaGrt= TotOpx=	a + (Al	0 /2). XFe 0 0.062 1.02	
TITLE = ModeGrt= XFeGrt= XFeDpx= XFeBT= XFeCrd= XAnPI=	MODEL 3 XA 10 0.603 0.43 0 0.361 DNVERGED P-	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPl=	40 0.278 0.49 0 0 0.593	/ sumwhere ModeBt= XMnGrt= XAIOpx= XAIBt= XMnCRD =	sum = Fe2+ + 0 0.057 0.057 0 0 0	ModeCrd= XcaGrt= TotOpx=	a + (Al	0 /2). XFe 0 0.062 1.02	20px = Fe2+/sum DIFFERENCE 0.38 KB
TITLE = ModeGrt= XFeGt= XFeOpx= XFeBT= XFeCrd= XAnPI= INITIAL AND CO	MODEL 3 XA 10 0.603 0 0.361 DNVERGED P- CONVEI 1030 C	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A RGED(FINAL)	40 0.278 0.49 0 0 0.593	/ sumwhere ModeBt= XMnGrt= XAI0px= XAIBt= XMnCRD =	sum = Fe2+ + 0 0.057 0.057 0 0 0 0 1 0 0 0	ModeCrd= XcaGrt= TotOpx=		0 /2). XFe 0 0.062 1.02 0	DIFFERENCE
TITLE = ModeGrt= XFeGrt= XFeDpx= XFeBT= XFeCrd= XAnPI= INITIAL AND CO Fe AI GOPQ GrtDpx GOPQ GrtBt GOPQ	MODEL 3 XA 10 0.603 0.43 0 0 0.361 DNVERGED P- CONVEI 1030 C 1030 C 0 C	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A GED(FINAL) 9.95 KB 9.95 KB	40 0.278 0.49 0 0 0.593	c / sumwhere ModeBt= XMnGrt= XAIBt= XMnCRD = AL COMPOSIT 965C 787 C O C	sum = Fe2+ + 0 0.057 0.057 0 10NS INITIAL 9.56(8 7.02 KB 0.00 KB	ModeCrd= XcaGrt= TotOpx=	66C 244C 0C	0 /2). XFe 0 0.062 1.02 0	DIFFERENCE 0.38 KB 2.93 KB 9.95 KB
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TITLE = ModeGrt= XFeGt= XFeOt= XFeBT= XFeCtd= XAnPl= INITIAL AND CO Fe AI GOPQ GrtDpx GOPQ GrtDpx GOPQ GrtCrd GOPQ M/FM rock	MODEL 3 XA 10 0.603 0.43 0 0.361 20NVERGED P- CONVEI 1030 C 1030 C 1030 C 0 C 0 C 0 C	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A GED(FINAL) 9.95 KB 9.95 KB	40 0.278 0.49 0 0 0.593	/ sumwhere ModeBt= XMnGrt= XAIOpx= XAIOpx= XAIOpx= XAIOpx= XAIOpx= AL COMPOSIT 965C 787 C 0 C 0 C 0 C	sum = Fe2+ + 0 0.057 0.057 0 0 10NS INIT/AL 9.56KB 7.02 KB 0.00 KB	ModeCrd= XcaGrt= TotOpx=	66C 244C 0C	0 /2). XFe 0.062 1.02 0	DIFFERENCE 0.38 KB 2.93 KB 9.95 KB
TITLE = ModeGrt= XFeGt= XFeOt= XFeBT= XFeCd= XAnPI= INITIAL AND CO Fe AI GOPQ GrtDpx GOPQ GrtBt GOPQ GrtBt GOPQ M/FM rock M/FM Grt	MODEL 3 XA 10 0.603 0.43 0 0 0 0 0.361 DNVERGED P- CONVEI 1030 C 1030 C 0 C 0 C	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A GED(FINAL) 9.95 KB 9.95 KB	40 0.278 0.49 0 0 0.593	C / sumwhere ModeBt= XMnGrt= XAIOpx= XAIOpx= XAIOpx= XAIOpx= AL COMPOSIT 965C 787 C 0 C	Sum = Fe2+ + 0.057 0.057 0 0 10NS 1NITIAL 9.56KB 7.02 KB 0.00 KB	ModeCrd= XcaGrt= TotOpx=	66C 244C 0C	0 /2). XFe 0.062 1.02 0	DIFFERENCE 0.38 KB 2.93 KB 9.95 KB
TITLE = ModeGrt= XFeGt= XFeOt= XFeBT= XFeCrd= XAnPl= INITIAL AND CO Fe AI GOPQ GrtOpx GOPQ GrtOpx GOPQ GrtCrd GOPQ M/FM rock	MODEL 3 XA 10 0.603 0.43 0 0.361 20NVERGED P- CONVEI 1030 C 0 C 0 C 0 C 0 C 0 C 0 C 0.495 0.371	ModeOpx= XMgGrt= XMgOpx= XMgBt= XMgCrd= XAbPI= T ESTIMATES A GED(FINAL) 9.95 KB 9.95 KB	40 0.278 0.49 0 0 0.593	C / sumwhere ModeBt= XMI0frt= XAI0px= XAI0t= XAI XAI XAI XAI XAI XAI XAI XAI XAI XAI	sum = Fe2+ + 0.057 0.057 0 10NS INITIAL 9.56KB 7.02 KB 0.00 KB	ModeCrd= XcaGrt= TotOpx=	66C 244C 0C	0 /2). XFe 0 0.062 1.02 0	DIFFERENCE 0.38 KB 2.93 KB 9.95 KB
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