



P-T-H₂O-CO₂-O₂ calculations in metamorphic rocks using EXCEL

by B. D. GOSCOMBE

The following is a near comprehensive list of geothermometers, geobarometers, and O₂ and H₂O activity calculations available in the literature up to May 1992. I have programmed a lot of these on EXCEL files, but most have not been rigorously checked. Consequently I do not want to release these for general use as yet. However if you need to use any specific calculations in this list get in contact with me (send a 3.5" DD disc) and I will tidy up and test those specific calculations and send them to you as soon as I can.

Note that I have indicated the calibrations which are not available on my EXCEL files, and the ones which I have not been able to get to work as yet. Those listed without any comment are available on my EXCEL files. I have included the entire list of what is available in the literature (references for all these are also given).

Also included are the calibrations which also have available the option of using a graphical determination of the result. For most (but not all) of these, the parameters which are required for plotting can be calculated from my EXCEL files.

Also listed are the models available in the literature and from Tim Holland and Roger Powell (pers. comm., 1988) for calculating mineral end-member activities (only plagioclase and garnet are calculated using non-ideal activity models). These are particularly useful if using THERMOCALC (Powell and Holland, 1988).

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THERMOMETRY

GARNET-BIOTITE

Garn-bio

Perchuk 67
Goldman & Albee 77
Ferry & Spear 78
Perchuk 81
Perchuk & Lavrent'eva 83
Hodges & Spear 82
Indare & Martignole 85a,b
Dachs 90
William & Grambling 90
Ganguly & Saxena 84
Dasgupta et al 91
Perchuk et al 85
Ghent & Stout 81 (in P-file)
Hodges & Crowley 85
(in P-file, from Dachs 90)

graph

Garn-bio-mu-pl

GARNET-MUSCOVITE

Garn-musc

Krogh & Raheim 78
Green & Hellman 82
Hynes & Forest 88

GARNET-CHLORITE

Garn-chlor

Grambling 90
Dickenson & Hewitt 86
also modified by Laird 89
Ghent et al 87 (in Laird 89)

graph
correct
correct
correct

GARNET-ORTHOPYROXENE

Garn-opx

Powell 78
Dahl 80
Harley 84
Sen & Bhattacharya 84
Bhattacharya et al 91
Perchuk et al 85

N/A

GARNET-CLINOPYROXENE

Garn-cpx

Raheim & Green 74
Ganguly 79
Ellis & Green 79
Dahl 80
Powell 85
Sengupta et al 89
Krogh 88
Pattison & Newton 89

GARNET-CORDIERITE-(sill)

Garn-cord-(sill)	Thompson 76	graph
	Lonker 81	graph
	Martignole & Sisi 81	graph
	Perchuk & Lavrent'eva 83	graph
	Bhattacharya etal 88	
	Perchuk etal 85	
	Nichols etal 92 (Contrib.Min.Pet.)	N/A

GARNET-STAUROLITE-(sill)

Garn-staur-(sill)	Hutcheon 79	
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GARNET-HORNBLLENDE

Garn-horn	Graham & Powell 84	graph
	Perchuk etal 85	graph

GARNET-ILMENITE

Garn-ilm	Pownceby etal 87	correct
	Pownceby etal 91	correct

ORTHOPYROXENE-CLINOPYROXENE+HORN+BIQ

Opx-cpx	Wood & Banno 73	
	Wells 77	
	Kretz 82	
	Lindsley 83 (igneous only)	N/A
	Nickel etal 85	graph
	Gasparik 84	graph
Opx-horn	Perchuk etal 85	graph
Cpx-horn	Perchuk etal 85	graph
Cpx-bio	Perchuk etal 85	graph

ORTHOPYROXENE-BIOTITE

Opx-bio	Sengupta etal 90	
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ILMENITE-ORTHOPYROXENE / CLINOPYROXENE

Ilm-opx	Bishop 80	
Ilm-cpx	Bishop 80	

ILMENITE-MAGNETITE

Ilm-mag	Buddington & Lindsley 64	graph
	Spencer & Lindsley 81	graph
	Andersen & Lindsley 88	graph
	Powell & Powell 77a	graph

<u>PLAGIOCLASE-MUSCOVITE-(sill)</u>		
Plag-musc-(sill)	Cheney & Guidotti 79	correct
	Green & Usdansky 86	correct
	Hodges & Spear 82	N/A
<u>PLAGIOCLASE-K-FELDSPAR</u>		
Plag-Kfld	Stormer 75	graph
	Whitney & Stormer 77	graph
	Powell & Powell 77	graph
	Brown & Parsons 81	graph
	Fuhrman & Lindsley 88	N/A
<u>PLAGIOCLASE-HORNBLLENDE</u>		
Plag-horn	Spear 81	graph
	Blundy & Holland 90	
<u>PLAGIOCLASE-SCAPOLITE</u>		
Plag-scap	Goldsmith & Newton 77	graph
<u>TOURMALINE-BIOTITE</u>		
Tourm-bio	Colopietro & Friberg 87	
<u>BIOTITE-MUSCOVITE / CHLORITE</u>		
Bio-musc	Hoisch 89	
Bio-chlor	Dickenson pers. (Laird 89)	
<u>SPINEL-CORDIERITE</u>		
Spin-cord	Vielzeuf 83	graph
	Nichols etal 92 (Contrib.Min.Pet.)	N/A
Spin-cord-garn	Nichols etal 92 (Contrib.Min.Pet.)	N/A
<u>SPINEL-SAPPHIRINE</u>		
Spin-sapp	Owen & Greenough 91	
<u>OLIVINE ± GARN ± ILM ± OPX ± SPIN</u>		
Olivine-garn	Griffin etal 89	N/A
	O'Neil & Wood 79	correct
Olivine-ilm	Andersen & Lindsley 81	correct
Olivine-opx-sp	Witt-Eickchen & Seck 91	correct
<u>CALCITE-(DOLOMITE)</u>		
CC-dol	Powell etal 84	graph
	Anovitz & Essene 87	graph
	Bickle & Powell 77	graph
	Dachs 90	graph
<u>OTHERS</u>		
Illite	many, see J.Meta.Geol. 1992#1	N/A
Chlorite	Authors unknown	N/A

BAROMETRY

GARNET-ILM-RUT ± PLAG ± (TITANITE-ZOISITE)

Gn-ilm-rut-(sill)	Bohlen etal 83	graph
Gn-ilm-rut-pl-(sill)	Bohlen & Liotta 86	graph
Titan-pl-rut-(ky)	Manning & Bohlen 91	graph
Titan-zo-gn-(rt,q)	Manning & Bohlen 91	graph
Titan-gn-(rt,q,ky)	Manning & Bohlen 91	graph

GARNET-PLAGIOCLASE-OPX-(q)

Gn-opx-pl-(q)	Rollinson 81	
	Perkins & Newton 81	
	Newton & Perkins 82	
	Newton 83	
	Perkins & Chipera 85	graph
	Eckert etal 91 (89 abst)	correct
	Bhattacharya etal 91	
	Bohlen etal 83a	graph
	Powell & Holland 88	graph

GARNET-PLAGIOCLASE-OPX-CPX

Gn-opx-cpx-pl	Hansen 81
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GARNET-PLAGIOCLASE-CPX (or OPX)

Gn-cpx-pl-(q)	Ghent etal 83	
	Perkins & Newton 81	
	Newton & Perkins 82	
	Newton 83	
	Moecher etal 88	graph
	Eckert etal 91	
	Powell & Holland 88	graph
Gn-opx-plag-(q)	Moecher etal 88	graph

GARNET-ORTHOPYROXENE (Al-exchange)

Gn-opx	Wood & Banno 73	N/A
	Harley & Green 82	
	Harley 84	
	Perchuk etal 85	

GARNET-PLAGIOCLASE-(sill/ky, q)

Gn-pl-(sill/ky,q)	Ghent 76	
	Newton & Hasleton 81	
	(and Newton 83)	
	Harris & Jayaram 82	
	Edward & Essene 88	graph
	Koziol & Newton 88	
	McKenna & Hodges 88	correct
	Dachs 90	correct
	Hodges & Spear 82	
	Ganguly & Saxena 84	
	Hodges & Crowley 85	correct
	Koziol 89 (Koziol & Newton 88)	N/A
	Kohn & Spear 91 (not new)	N/A
	Perchuk et al 85	
	Powell & Holland 88	graph

GARNET-PLAGIOCLASE + MUSC + BIO ± (q)

Gn-pl-mu-bi-(q)	Ghent & Stout 81	
	Hoisch 90 (Mg)	
	Hodges & Crowley 85	
	(from Dachs 90)	
	Hoisch 91 (Mg)	correct
Gn-pl-mu-bi	Hodges & Spear 82 (Fe,Mg)	
	Powell & Holland 88	graph
	Hoisch 90 (Fe, Mg)	
	Hoisch 91 (Fe,Mg)	correct
Gn-pl-bi	Hoisch 90 (Fe, Mg)	
	Hoisch 91 (Fe,Mg)	correct
Gn-pl-mu	Hoisch 90 (Mg)	
	Hoisch 91 (Mg)	correct
	Hodges & Crowley 85	correct

GARNET-MUSCOVITE + BIOTITE-(sill,q)

Gn-mu-bi-(sill/ky,q)	Hodges & Crowley 85	
	Holdaway et al 88	
	Spear & Selverstone 83	N/A
	Robinson 83	N/A
Gn-mu-(sill/ky,q)	Hodges & Crowley 85 (is T)	correct

CORDIERITE ± OPX ± GARN ± SPIN ± (sill/q/co)

Cord-gn-(sill-q)	Hutcheon etal 74	graph
	Holdaway & Lee 77	graph
	Newton & Wood 79	graph
	Lonker 81	graph
	Martignole & Sisi 81	graph
	Thompson 76	
	Harris & Holland 84	graph
	Bhattacharya 86	
Cord-sp-(co or sill)	Perchuk etal 85	
	Harris 81	
Cord-sp-(q)	Vielzeuf 83	
	Bhattacharya 86	
Cord-sp-gn-(sill)	Harris 81	
	Bhattacharya 86	
Cord-sp-opx-(sill)	Nichols etal 92 (Contrib.Min.Pet.)	N/A
	Harris & Holland 84	graph
Cord-opx-(sill-q)	Harris & Holland 84	graph
	Bhattacharya 86	
Cord-opx-(q)	Perchuk etal 85	
Cord-opx-gn-(q)	Harris & Holland 84	graph
	Bhattacharya 86	
Sp-gn-(sill-q)	Bohlen, Dollase & Wall 86	graph N/A
Sp-gn-(sill-co)	Bohlen, Dollase & Wall 86	graph N/A

BIOTITE-MUSCOVITE ± CHLORITE ± KFELDSPAR

Bi-mu-chl±Kfld	Powell & Evans 83	graph, correct
	Dachs 90	correct
	Bucher-Nurminen 87	graph, correct
Bi-mu-Kfld	Powell & Evans 83	graph, correct
	Bucher-Nurminen 87	graph
Phengite-(bi,q,kfld)	Massone & Schreyer 87	graph N/A

HORNBLende-GARN-PLAG ± CHL (HORN only)

Gn-hn-pl	Kohn & Spear 89	graph, correct
	Kohn & Spear 90	graph
Horn-in granodiorite	Rutter etal 89	graph
	Hammarstrom & Zen 86	graph
	Hollister etal 87	graph
	Johnson & Rutherford 89	graph
	Schmidt 92	graph
Horn-chlor	Laird 89	

OLIVINE+CPX+OPX+GARN+PLAG

Olivine-opx	Bohlen & Boettcher 81	graph, correct
	Newton 83	correct
Olivine-pl-gn	Newton 83	correct
	Bohlen etal 83a	graph, N/A
Olivine-cpx	Adams & Bishop 86	correct
Cpx-pl	Rollinson 81	correct
Cpx-gn	Mukhopadhyay 91	N/A
Albite-jadeite	Newton 83	correct
	Holland 80	N/A
	Gasparik & Lindsley 80	N/A

OTHERS

Sphalerite-(py-pyrr)	Scott 76	graph, N/A
	Toulmin etal 91	graph, N/A

WATER BAROMETRY

GARNET-STAUROLITE/CHLORITE-(sill,q)

Staur-garn-(sill,q)	Holdaway etal 88	N/A
Garn-chlor	Author unknown	N/A

GARNET-CORDIERITE-(sill)

Garn-cord-(sill)	Holdaway & Lee 77	graph, N/A
	Newton & Wood 79	graph, N/A
	Lonker 81	graph, N/A
	Martignole & Sisi 81	graph, N/A
	Bhattacharya & Sen 85	correct

GARNET-BIOTITE-K-FELDSPAR-(sill+cd)

Gn-bi-Kfld-(sill,cd)	Phillips 80	correct
Gn-bi-Kfld-(sill,q)	Edwards & Essene 88	graph, correct
	Perchuk etal 85	N/A
	Perchuk etal 85 (2nd)	N/A

BIOTITE-MAGNETITE-K-FELDSPAR

Bio-mag-Kfld(Na)	Wones & Eugster 65	correct
	Wones 71	N/A
	Wones 81	N/A
	(both in Dawes & Evans 91)	

MUSCOVITE-K-FELDSPAR-(sill)

Musc-Kfld-(sill)	Edwards & Essene 88	graph
	Holdaway etal 88	N/A

ORTHOPYROXENE-BIOTITE-K-FELDSPAR-(q)

Opx-bi-Kfld-(q)	Lamb & Valley 88	graph, correct
	Edwards & Essene 88	graph, N/A
	Bohlen etal 83	N/A
	Moecher & Essene 91	N/A

ALBITE-PARAGONITE-(sill)

Albite-parag-(sill)	Triboulet & Audren 85	
	(Eugster etal 72, activity)	correct
	(Chatterjee & G 79, activity)	
	(Pigage & Greenwood 82, activity)	
	Sevigny & Ghent 89	N/A

HORNBLLENDE-OPX-CPX

Hn-opx-cpx	Phillips 80	graph, correct
	Jenkins 88	N/A
	Lamb & Valley 88	graph, correct

PLAGIOCLASE-GARN-SCAP-CLINOZOISITE-(woll, cc, q)

Pl-gn-clinozois-(q)	Moecher & Essene 91 (H2O)	N/A
Pl-gn-scap-(q)	Moecher & Essene 91 (CO2)	N/A
Pl-gn-(cc, q, woll)	Perchuk etal 85 (CO2)	N/A

OXYGEN FUGACITY

MAGNETITE-ILMENITE (see T-file)

Mag-ilm	Buddington & Lindsley 64	graph
	Spencer & Lindsley 81	graph
	Andersen & Lindsley 88	graph
	Powell & Powell 77a	graph
Mag-rut-ilm	Sevingny & Ghent 89	N/A

ORTHOPYROXENE-MAGNETITE

Opx-mag	Robinson etal 83	N/A
Opx-sp-ol	Ballhaus etal 91	N/A

GARNET-BIOTITE-MUSCOVITE-(mag, q)

Gn-bi-mu-(mag,q) Zen 85

GARNET-ILMENITE-(sill, q)

Gn-ilm-(q, sill) Bhattacharya & Sen 86

COMMENTS.

graph	The result can also be obtained graphically using the original publication.
N/A	Not available on EXCEL programs.
correct	Has not been programed on EXCEL correctly.
minerals in brackets	These phases must be in excess in the assemblage, quartz is in excess in most calculations but is not indicated in the listing above.

MINERAL ABBREVIATIONS.

garn, gn	garnet	bio, bi	biotite
mu, musc	muscovite	chlor, chl	chlorite
pl, plag	plagioclase	opx	orthopyroxene
cpx	clinopyroxene	cord, cd	cordierite
sill, si	sillimanite	staur	staurolite
horn, hn	hornblende	ilm	ilmenite
mag	magnetite	Kfld	K-feldspar
scap	scapolite	tourm	tourmaline
spin, sp	spinel	sapp	sapphirine
cc	calcite	dol	dolomite
rut, rt	rutile	titan	titanite (sphene)
ky	kyanite	zo	zoisite
q	quartz	co	corundum
py	pyrite	pyrr	pyrrhotite
parag	paragonite	clinozois	clinozoisite
woll	wollastonite	ol	olivine

MINERAL ACTIVITY CALCULATIONS

using EXCEL

<u>PLAGIOCLASE</u>	Newton etal 80 (after Kerrick & Darken 75) Newton 83 Elkins & Grove 90 Green & Usdansky 86	correct correct
<u>GARNET</u>	Newton & Hasleton 81 (Hodges & Spear 82, Powell pers. comm.) Ganguly & Saxena 84 Ganguly & Kennedy 74 Newton & Perkins 82 Berman 90 Perchuk etal 85	N/A N/A
<u>CLINOPYROXENE</u>	Holland 90 Powell & Holland pers. com.	N/A
<u>ORTHOPYROXENE</u>	Holland 90 Perchuk etal 85 Powell & Holland pers. com.	N/A N/A
<u>CORDIERITE</u>	Perchuk etal 85 Powell & Holland pers. com.	N/A
<u>MUSCOVITE</u>	Powell & Evans 83 Powell & Holland pers. com.	
<u>BIOTITE</u>	Perchuk etal 85 Powell & Holland pers. com.	N/A
<u>AMPHIBOLE</u>	Powell & Holland pers. com.	
<u>SPINEL</u>	Powell & Holland pers. com.	
<u>CHLORITE</u>	Powell & Holland pers. com.	
<u>EPIDOTE</u>	Powell & Holland pers. com.	

P-T-H₂O-CO₂-O₂ CALCULATIONS

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