REM" THIS VERSION OF RCLC IS A MODIFIED VERSION OF TOM CHACKO'S 1996 ORIGINAL."

REM" THE MODIFICATIONS HAVE BEEN MADE BY CHRIS MCFARLANE (04-97), "

REM" DAVID PATTISON (05-97 AND 10-01) AND TOM CHACKO (05-02)."

REM" "

REM" RCLC CALCULATES P AND T FROM GRT-PL-OPX-QTZ EQUILIBRIA (GRT-OPX-PL-QTZ BAROMETER"

REM" AND GRT-OPX AL-IN-OPX THERMOMETER), CORRECTED FOR LATE FE-MG EXCHANGE. "

REM" "

REM" FE-MG RATIOS OF GRT, OPX, BT AND CRD ARE ADJUSTED ACCORDING TO THEIR MODES"

REM" TO SATISFY GRT-OPX, GRT-CRD & GRT-BT FE-MG EXCHANGE EQUILIBRIA."

REM" "

REM" ALL THERMODYNAMIC DATA (END-MEMBERS AND SOLUTION MODELS) ARE FROM"

REM" TWQ202b (FILES BA96A.DAT AND BA96A.SLN), EXCEPT FOR BT WHICH USES"

REM" THE SOLUTION MODEL OF MCMULLIN (1991, CAN. MINERAL.). FOR REFS, SEE BERMAN (1991,

REM" CAN. MINERAL.), BERMAN AND ARANOVICH (1996, CONTRIB. MINERAL. PETROL.) AND"

REM" ARANOVICH AND BERMAN (1997, AM. MINERAL.)"

REM" "

REM" REQUIRED INPUT DATA ARE CATIONS IN GARNET (12 OXYGENS), OPX (6 OXY), CRD"

REM" (18 OXY), BT (11 OXY) AND PL (8 OXY), AND MODAL PROPORTIONS OF GRT, OPX,"

REM" CRD AND BT. IF THERE IS NO CRD OR BT, ZEROES ARE INSERTED AND THE PROGRAM STILL WORKS."

REM" IF OPX ANALYSES ARE NOT RECALCULATED FOR FE3+, REPORT TOTAL IRON AS FE2+ IN THE INPUT FILE."

BEGIN:

CLS

CLEAR

REM"READ IN THERMODYNAMIC DATA - TWQ202B DATA SET (BA96A.DAT) OF BERMAN."

DIM DATASET(12, 6)

FOR J = 1 TO 12

 FOR I = 1 TO 6

 READ DATASET(J, I)

 NEXT I

NEXT J

PRINT "RCLC - GRT-OPX-PL-QTZ P-T ESTIMATES CORRECTED FOR LATE FE-MG EXCHANGE"

PRINT ""

SAMPLE:

ANSWER1$ = "Z"

CLOSE #1

CLOSE #2

REM "TYPE IN INPUT FILENAME AND SHORT DESCRIPTION OF SAMPLE"

REM "INPUT FILENAME HAS NO SUFFIX (E.G., C10B RATHER THAN C10B.IN)

PRINT ""

INPUT "TYPE IN FILE TO READ (E.G., C10B):"; FILEIN$

OPEN FILEIN$ FOR INPUT AS #1

FILEOUT$ = FILEIN$ + ".RC"

OPEN FILEOUT$ FOR OUTPUT AS #2

PRINT ""

PRINT "TYPE IN A TITLE OR SHORT DESCRIPTION OF THE SAMPLE"

PRINT ""

INPUT TITLE$

REM "FORMAT OF INPUT DATA"

INPUT #1, SAMPLE$, FEGAR$, MNGAR$, MGGAR$, CAGAR$, MODEGAR$

INPUT #1, GAR$, FEGAR, MNGAR, MGGAR, CAGAR, MODEGAR

INPUT #1, OPX$, SIOPX$, TIOPX$, ALOPX$, CROPX$, Fe3OPX$, FE2OPX$, MNOPX$, MGOPX$, CAOPX$, MODEOPX$

INPUT #1, OPX$, SIOPX, TIOPX, ALOPX, CROPX, Fe3OPX, FE2OPX, MNOPX, MGOPX , CAOPX , MODEOPX

INPUT #1, CRD$, FECRD$, MNCRD$, MGCRD$, MODECRD$

INPUT #1, CRD$, FECRD, MNCRD, MGCRD, MODECRD

INPUT #1, BT$, SIBT$, TIBT$, ALBT$, FEBT$, MNBT$, MGBT$, NABT$, KBT$, MODEBT$

INPUT #1, BT$, SIBT, TIBT, ALBT, FEBT, MNBT, MGBT, NABT, KBT , MODEBT

INPUT #1, PLAG$, CA$, NA$, K$

INPUT #1, PLAG$, CA, NA, KPL

MODEL:

REM "OPX MOLE FRACTION OPTIONS AND CALCULATIONS"

 PRINT ""

 PRINT "YOU HAVE A CHOICE FOR CALCULATING XALM IN OPX."

 PRINT "THE FOLLOWING FORMULAE ASSUME A 6-OXYGEN OPX FORMULA."

 PRINT ""

 PRINT "1: XALM = Al - (2 - Si)"

 PRINT "2: XALM = Al/2 "

 PRINT "3: XALM = (Al/2) / (Fe2+ + Mg + Mn + Ca + (Al/2) )"

 PRINT "4: XALM = (Al - Fe3+ - Cr - (2\*Ti) ) / 2"

 PRINT ""

 INPUT "PLEASE ENTER 1,2,3,4: ", NUM$

 IF NUM$ = "1" THEN GOSUB ALOPX1:

 IF NUM$ = "2" THEN GOSUB ALOPX2:

 IF NUM$ = "3" THEN GOSUB ALOPX3:

 IF NUM$ = "4" THEN GOSUB ALOPX4:

 XFEOPXI = XFEOPX

 MGRATIOOPX = MGOPX / (MGOPX + FE2OPX)

 MGRATIOOPXI = MGRATIOOPX

 FERATIOOPX = 1 - MGRATIOOPX

 TOTOPX = XFEOPX + XMGOPX + XALM1+(TIOPX/2)+(Fe3OPX/2)+(CROPX/2)+(MNOPX/2)+(CAOPX/2)

REM "GARNET MOLE FRACTION CALCULATIONS"

 XMGGAR = MGGAR / (MGGAR + CAGAR + FEGAR + MNGAR)

 XFEGAR = FEGAR / (MGGAR + CAGAR + FEGAR + MNGAR)

 XCAGAR = CAGAR / (MGGAR + CAGAR + FEGAR + MNGAR)

 XMNGAR = MNGAR / (MGGAR + CAGAR + FEGAR + MNGAR)

 XFEGARI = XFEGAR

 MGRATIOGAR = MGGAR / (MGGAR + FEGAR)

 MGRATIOGARI = MGRATIOGAR

 MODXCAGAR = (CAGAR + MNGAR) / (CAGAR + MNGAR + FEGAR + MGGAR)

REM "BIOTITE MOLE FRACTION CALCULATIONS"

 IF MODEBT < 0.01 THEN

 XFEBT = 0

 XMGBT = 0

 XTIBT = 0

 XALBT = 0

 MGRATIOBT = 0

 ELSE

 ALIVBT = 4.0 - SIBT

 ALVIBT = ALBT - ALIVBT

 XFEBT = FEBT/ (FEBT+MGBT+ALVIBT+TIBT+MNBT)

 XMGBT = MGBT/ (FEBT+MGBT+ALVIBT+TIBT+MNBT)

 XALBT = ALVIBT/(FEBT+MGBT+ALVIBT+TIBT+MNBT)

 XTIBT = TIBT/ (FEBT+MGBT+ALVIBT+TIBT+MNBT)

 MGRATIOBT = MGBT / (MGBT + FEBT)

 END IF

 XFEBTI = XFEBT

 MGRATIOBTI = MGRATIOBT

REM "CORDIERITE MOLE FRACTION CALCULATIONS"

 IF MODECRD < 0.01 THEN

 XFECRD = 0

 XMGCRD = 0

 XMNCRD = 0

 MGRATIOCRD = 0

 ELSE

 XFECRD = FECRD / (FECRD + MGCRD + MNCRD)

 XMGCRD = MGCRD / (FECRD + MGCRD + MNCRD)

 XMNCRD = MNCRD / (FECRD + MGCRD + MNCRD)

 MGRATIOCRD = MGCRD / (MGCRD + FECRD)

 END IF

 MGRATIOCRDI = MGRATIOCRD

 XFECRDI = XFECRD

REM "PLAGIOCLASE MOLE FRACTIONS"

 XAN = CA / (CA + NA + KPL)

 XAB = NA / (NA + CA + KPL)

 XORT = KPL / (NA + CA + KPL)

IF ANSWER1$ = "y" OR ANSWER1$ = "Y" THEN GOTO APRINT

PRINT #2, "RCLC: GRT-OPX-PL-QTZ P-T ESTIMATES CORRECTED FOR LATE FE-MG EXCHANGE"

PRINT #2, " THERMODYNAMIC DATA AND EXPRESSIONS FROM TWQ202B"

PRINT #2, ""

PRINT #2, FILEIN$;": "; TITLE$

PRINT #2, ""

APRINT:

IF ANSWER1$ = "y" OR ANSWER1$ = "Y" THEN PRINT #2," "

IF ANSWER1$ = "y" OR ANSWER1$ = "Y" THEN PRINT #2," "

PRINT #2, ALCHOICE$

PRINT #2, ALCHOICE2$

PRINT #2, ""

PRINT #2, USING "ModeGrt = ##.## ";MODEGAR; USING " ModeOpx = ##.## ";MODEOPX; USING " ModeBt = ##.## "; MODEBT; USING " ModeCrd = ##.## "; MODECRD

PRINT #2, USING "XFeGrt = #.### "; XFEGAR; USING " XMgGrt = #.### "; XMGGAR; USING " XMnGrt = #.### "; XMNGAR; USING " XCaGrt = #.### "; XCAGAR

PRINT #2, USING "XFeOpx = #.### "; XFEOPX; USING " XMgOpx = #.### "; XMGOPX; USING " XAlOpx = #.### "; XALM1 ; USING " TotOpx = #.### "; TOTOPX

IF MODEBT > 0.01 THEN PRINT #2, USING "XFeBt = #.### "; XFEBT; USING " XMgBt = #.### "; XMGBT ; USING " XAlBt = #.### "; XALBT ; USING " XTiBt = #.### "; XTIBT

IF MODECRD> 0.01 THEN PRINT #2, USING "XFeCrd = #.### "; XFECRD; USING " XMgCrd = #.### "; XMGCRD; USING " XMnCrd = #.### "; XMNCRD

PRINT #2, USING "XAnPl = #.### "; XAN; USING " XAbPl = #.### "; XAB; USING " XOrPl = #.### "; XORT

REM " VOLUME FRACTIONS OF FE-MG MINERALS FROM MODE"

VFGAR = MODEGAR / (MODEGAR + MODEOPX + MODECRD + MODEBT)

VFOPX = MODEOPX / (MODEGAR + MODEOPX + MODECRD + MODEBT)

VFCRD = MODECRD / (MODEGAR + MODEOPX + MODECRD + MODEBT)

VFBT = MODEBT / (MODEGAR + MODEOPX + MODECRD + MODEBT)

REM "CONVERT VOLUME FRACTION MINERALS TO MOLE FRACTION MINERALS"

REM "DENSITIES"

DENSFEGAR = 4.33

DENSMGGAR = 3.54

DENSCAGAR = 3.56

DENSMNGAR = 4.19

DENSFEOPX = 3.96

DENSMGOPX = 3.21

DENSMGCRD = 2.53

DENSFECRD = 2.78

DENSFEBT = 3.3

DENSMGBT = 2.7

DENSGAR = (DENSFEGAR \* XFEGAR) + (DENSMGGAR \* XMGGAR) + (DENSCAGAR \* XCAGAR) + (DENSMNGAR \* XMNGAR)

DENSOPX = (DENSFEOPX \* (1 - MGRATIOOPX)) + (DENSMGOPX \* MGRATIOOPX)

DENSCRD = (DENSFECRD \* (1 - MGRATIOCRD)) + (DENSMGCRD \* MGRATIOCRD)

DENSBT = (DENSFEBT \* (1 - MGRATIOBT)) + (DENSMGBT \* MGRATIOBT)

REM "MOLECULAR WEIGHTS"

MWOPX = (SIOPX \* 28.1) + (TIOPX\*47.9) + (ALOPX \* 26.1) + (CROPX\*52!) + (Fe3OPX\*55.8) + (FE2OPX \* 55.8) + (MGOPX \* 24.3) + (MNOPX \* 54.9) + (CAOPX \* 40.1) + (6 \* 16)

MWGAR = (3.00 \* 28.1) + (2.00 \* 26.1) + (FEGAR \* 55.8) + (MGGAR \* 24.3) + (MNGAR \* 54.9) + (CAGAR \* 40.1) + (12 \* 16)

MWCRD = (5.00 \* 28.1) + (4.00 \* 26.1) + (FECRD \* 55.8) + (MGCRD \* 24.3) + (MNCRD \* 54.9) + (18 \* 16)

MWBT = (SIBT \* 28.1) + (TIBT \* 47.9) + (ALBT \* 26.1) + (FEBT \* 55.8) + (MNBT \* 54.9) + (MGBT \* 24.3) + (NABT \* 23) + (KBT \* 39.1) + (11 \* 16) + 2

REM "MOLES OF MINERALS AND MOLES OF FE-MG COMPONENTS OF MINERALS"

MOLEGAR = (VFGAR \* DENSGAR) / MWGAR

MOLEOPX = (VFOPX \* DENSOPX) / MWOPX

IF MODECRD < 0.01 THEN

 MOLECRD = 0

ELSE

 MOLECRD = (VFCRD \* DENSCRD) / MWCRD

END IF

IF MODEBT < 0.01 THEN

 MOLEBT = 0

ELSE

 MOLEBT = (VFBT \* DENSBT) / MWBT

END IF

MOLEFEMGGAR = MOLEGAR \* (FEGAR + MGGAR)

MOLEFEMGOPX = MOLEOPX \* (FE2OPX + MGOPX)

MOLEFEMGCRD = MOLECRD \* (FECRD + MGCRD)

MOLEFEMGBT = MOLEBT \* (FEBT + MGBT )

REM "MOLE FRACTION OF FE-MG COMPONENTS OF MINERALS"

MFGAR = MOLEFEMGGAR / (MOLEFEMGGAR + MOLEFEMGOPX + MOLEFEMGCRD + MOLEFEMGBT)

MFOPX = MOLEFEMGOPX / (MOLEFEMGGAR + MOLEFEMGOPX + MOLEFEMGCRD + MOLEFEMGBT)

MFCRD = MOLEFEMGCRD / (MOLEFEMGGAR + MOLEFEMGOPX + MOLEFEMGCRD + MOLEFEMGBT)

MFBT = MOLEFEMGBT / (MOLEFEMGGAR + MOLEFEMGOPX + MOLEFEMGCRD + MOLEFEMGBT)

REM "CALCULATE XMG ROCK"

XMGROCK = (MGRATIOGAR \* MFGAR) + (MGRATIOOPX \* MFOPX) + (MGRATIOCRD \* MFCRD) + (MGRATIOBT \* MFBT)

XMGROCKI = XMGROCK

REM "CALCULATE GRT-OPX FE-MG - GRT-OPX-PL-QTZ (FE-END MEMBER)INTERSECTION"

REM "ASSUME INITIAL P-T TO BEGIN. ITERATE 10 TIMES."

TK = 1000

PBARS = 3000

P = 3

GOSUB CP

FOR J = 1 TO 10

 REM "CALCULATE GRT-OPX-PL-QTZ (FE-END MEMBER) PRESSURE"

 GOSUB BERMAN

 GOSUB FUHRMAN

 GOSUB ARANOVICH

 GOSUB VOLUMEPT

 DELTAHGAPES = (((3 \* HAN) + (6 \* HFS)) - ((3 \* HBQ) + (2 \* HALM) + HGR)) / 1000

 DELTASGAPES = (((3 \* SAN) + (6 \* SFS)) - ((3 \* SBQ) + (2 \* SALM) + SGR)) / 1000

 DELTAVGAPES = ((3 \* VAN) + (6 \* VFS)) - ((3 \* VBQ) + (2 \* VALM) + VGR)

 KGAPES = ((AAN ^ 3) \* (AFS ^ 6)) / (AGR \* (AAL ^ 2))

 P = ((TK \* DELTASGAPES) - DELTAHGAPES - (.008314 \* TK \* (LOG(KGAPES)))) / DELTAVGAPES

 PBARS = P \* 1000

 REM "CALCULATE GRT-OPX FE-MG EXCHANGE TEMP AT THIS PRESSURE"

 DELTAHFEMGOPX = (((1 \* HEN) + ((1 / 3) \* HALM)) - ((1 \* HFS) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGOPX = (((1 \* SEN) + ((1 / 3) \* SALM)) - ((1 \* SFS) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGOPX = ((1 \* VEN) + ((1 / 3) \* VALM)) - ((1 \* VFS) + ((1 / 3) \* VPY))

 GAMMAFEMGOPX = GAMMAGAR \* GAMMAOPX

 KDGAROPX = (XFEGAR \* XMGOPX) / (XMGGAR \* XFEOPX)

 TGAROPX = (DELTAHFEMGOPX + (P \* DELTAVFEMGOPX)) / (DELTASFEMGOPX - (.008314 \* LOG(KDGAROPX)) - (.008314 \* LOG(GAMMAFEMGOPX)))

 TK = TGAROPX

 TCGAROPX = TGAROPX - 273

 GOSUB CP

NEXT J

TGAROPXI = TCGAROPX

PFEMGGTOPI = P

IF MODECRD > 0.01 THEN

 REM "CALCULATE GRT-CRD FE-MG - GRT-OPX-PL-QTZ (FE END MEMBER) INTERSECTION"

 REM "ASSUME INITIAL P-T TO BEGIN. ITERATE 10 TIMES."

 TK = 1000

 PBARS = 3000

 P = 3

 GOSUB CP

FOR J = 1 TO 10

 REM "CALCULATE GRT-OPX-PL-QTZ (FE-END MEMBER) PRESSURE"

 GOSUB BERMAN

 GOSUB FUHRMAN

 GOSUB ARANOVICH

 GOSUB VOLUMEPT

 DELTAHGAPES = (((3 \* HAN) + (6 \* HFS)) - ((3 \* HBQ) + (2 \* HALM) + HGR)) / 1000

 DELTASGAPES = (((3 \* SAN) + (6 \* SFS)) - ((3 \* SBQ) + (2 \* SALM) + SGR)) / 1000

 DELTAVGAPES = ((3 \* VAN) + (6 \* VFS)) - ((3 \* VBQ) + (2 \* VALM) + VGR)

 KGAPES = ((AAN ^ 3) \* (AFS ^ 6)) / (AGR \* (AAL ^ 2))

 P = ((TK \* DELTASGAPES) - DELTAHGAPES - (.008314 \* TK \* (LOG(KGAPES)))) / DELTAVGAPES

 PBARS = P \* 1000

 REM "CALCULATE GRT-CRD FE-MG EXCHANGE TEMP AT THIS PRESSURE"

 GOSUB CORDIERITE

 DELTAHFEMGCRD = (((.5 \* HCRD) + ((1 / 3) \* HALM)) - ((.5 \* HFECRD) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGCRD = (((.5 \* SCRD) + ((1 / 3) \* SALM)) - ((.5 \* SFECRD) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGCRD = ((.5 \* VCRD) + ((1 / 3) \* VALM)) - ((.5 \* VFECRD) + ((1 / 3) \* VPY))

 GAMMAFEMGCRD = GAMMAGAR \* GAMMACRD

 KDGARCRD = (XFEGAR \* XMGCRD) / (XMGGAR \* XFECRD)

 TGARCRD = (DELTAHFEMGCRD + (P \* DELTAVFEMGCRD)) / (DELTASFEMGCRD - (.008314 \* LOG(KDGARCRD)) - (.008314 \* LOG(GAMMAFEMGCRD)))

 TK = TGARCRD

 TCGARCRD = TGARCRD - 273

 GOSUB CP

NEXT J

 TCGARCRDI = TCGARCRD

 PGARCRDI = P

ELSE

 TCGARCRD = 0

 TCGARCRDI = 0

 PGARCRD = 0

 PGARCRDI = 0

END IF

IF MODEBT > 0.01 THEN

 REM "CALCULATE GRT-BT FE-MG - GRT-OPX-PL-QTZ (FE END MEMBER) INTERSECTION"

 REM "ASSUME INITIAL P-T TO BEGIN. ITERATE 10 TIMES."

 TK = 1000

 PBARS = 3000

 P = 3

 GOSUB CP

FOR J = 1 TO 10

 REM "CALCULATE GRT-OPX-PL-QTZ (FE-END MEMBER) PRESSURE"

 GOSUB BERMAN

 GOSUB FUHRMAN

 GOSUB ARANOVICH

 GOSUB VOLUMEPT

 DELTAHGAPES = (((3 \* HAN) + (6 \* HFS)) - ((3 \* HBQ) + (2 \* HALM) + HGR)) / 1000

 DELTASGAPES = (((3 \* SAN) + (6 \* SFS)) - ((3 \* SBQ) + (2 \* SALM) + SGR)) / 1000

 DELTAVGAPES = ((3 \* VAN) + (6 \* VFS)) - ((3 \* VBQ) + (2 \* VALM) + VGR)

 KGAPES = ((AAN ^ 3) \* (AFS ^ 6)) / (AGR \* (AAL ^ 2))

 P = ((TK \* DELTASGAPES) - DELTAHGAPES - (.008314 \* TK \* (LOG(KGAPES)))) / DELTAVGAPES

 PBARS = P \* 1000

 REM "CALCULATE GRT-BT FE-MG EXCHANGE TEMP AT THIS PRESSURE"

 GOSUB MCMULLIN

 DELTAHFEMGBT = ((((1 / 3) \* HPHL) + ((1 / 3) \* HALM)) - (((1 / 3) \* HANN) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGBT = ((((1 / 3) \* SPHL) + ((1 / 3) \* SALM)) - (((1 / 3) \* SANN) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGBT = (((1 / 3) \* VPHL) + ((1 / 3) \* VALM)) - (((1 / 3) \* VANN) + ((1 / 3) \* VPY))

 GAMMAGARBT = GAMMABT \* GAMMAGAR

 KDGARBT = (XFEGAR \* XMGBT) / (XMGGAR \* XFEBT)

 TGARBT = (DELTAHFEMGBT + (P \* DELTAVFEMGBT)) / (DELTASFEMGBT - (.008314 \* LOG(KDGARBT)) - (.008314 \* LOG(GAMMAGARBT)))

 TK = TGARBT

 TCGARBT = TGARBT - 273

 GOSUB CP

NEXT J

 TCGARBTI = TCGARBT

 PGARBTI = P

ELSE

 TCGARBT = 0

 TCGARBTI = 0

 PGARBT = 0

 PGARBTI = 0

END IF

REM "CALCULATE CONVERGED INTERSECTION OF GRT-OPX AL-SOLUBILITY AND GRT-OPX-PL-QTZ USING"

REM "FE-END MEMBER EXPRESSIONS."

REM "CONVERGENCE APPROACH - 1. CALCULATE INITIAL INTERSECTION OF GRT-OPX AL-SOLUB"

REM "AND GRT-OPX-PL-QTZ."

REM "2. CHANGE KD GRT-OPX (AND IF APPLICABLE KD GRT-CRD AND KD GRT-BT) SO COINCIDES WITH 1.

REM "3. ADJUST FE/MG RATIOS OF FE-MG MINERALS TO SATIFY KD'S.

REM "4. REPEAT 10 TIMES (I = 1 TO 10) TO GET CONVERGENCE.

REM "ASSUME INITIAL TEMP TO BEGIN"

TK = 1000

PBARS = 3000

P = 3

FOR I = 1 TO 10

GOSUB CP

 REM "CALCULATE INTERSECTION OF FE-AL-OPX AND GRT-OPX-PL-QTZ IN 10 ITERATIONS (J = 1 TO 10)"

 FOR J = 1 TO 10

 REM "CALCULATE GRT-OPX-PL-QTZ (FE-END MEMBER) PRESSURE"

 GOSUB BERMAN

 GOSUB FUHRMAN

 GOSUB ARANOVICH

 GOSUB VOLUMEPT

 DELTAHGAPES = (((3 \* HAN) + (6 \* HFS)) - ((3 \* HBQ) + (2 \* HALM) + HGR)) / 1000

 DELTASGAPES = (((3 \* SAN) + (6 \* SFS)) - ((3 \* SBQ) + (2 \* SALM) + SGR)) / 1000

 DELTAVGAPES = ((3 \* VAN) + (6 \* VFS)) - ((3 \* VBQ) + (2 \* VALM) + VGR)

 KGAPES = ((AAN ^ 3) \* (AFS ^ 6)) / (AGR \* (AAL ^ 2))

 P = ((TK \* DELTASGAPES) - DELTAHGAPES - (.008314 \* TK \* (LOG(KGAPES)))) / DELTAVGAPES

 PBARS = P \* 1000

 REM "CALCULATE FE-ALOPX TEMPERATURE AT THIS PRESSURE"

 DELTAHFEAL = ((HALOPX + (3 \* HFS)) - HALM) / 1000

 DELTASFEAL = ((SALOPX + (3 \* SFS)) - SALM) / 1000

 DELTAVFEAL = (VALOPX + (3 \* VFS)) - VALM

 KFEAL = ((AFS ^ 3) \* AALOPX) / AAL

 TFEAL = (DELTAHFEAL + (P \* DELTAVFEAL)) / (DELTASFEAL - (.008314 \* LOG(KFEAL)))

 TK = TFEAL

 TC = TK - 273

 GOSUB CP

 NEXT J

IF I=1 THEN

 TFEALI = TC

 PFEALI = P

END IF

GOSUB BERMAN

GOSUB ARANOVICH

IF MODECRD > 0.01 THEN GOSUB CORDIERITE

IF MODEBT > 0.01 THEN GOSUB MCMULLIN

GOSUB VOLUMEPT

REM "CALCULATES A CORRECTED KD(GRT-OPX(FE-MG)) "

 DELTAHFEMGOPX = (((1 \* HEN) + ((1 / 3) \* HALM)) - ((1 \* HFS) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGOPX = (((1 \* SEN) + ((1 / 3) \* SALM)) - ((1 \* SFS) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGOPX = ((1 \* VEN) + ((1 / 3) \* VALM)) - ((1 \* VFS) + ((1 / 3) \* VPY))

 GAMMAFEMGOPX = GAMMAGAR \* GAMMAOPX

 KDGAROPX = ((TK \* DELTASFEMGOPX) - DELTAHFEMGOPX - (P \* DELTAVFEMGOPX) - (.008314 \* TK \* (LOG(GAMMAFEMGOPX)))) / (.008314 \* TK)

 KDGAROPX = EXP(KDGAROPX)

IF MODECRD > 0.01 THEN

REM "CALCULATES A CORRECTED KD(GRT-CRD) "

 DELTAHFEMGCRD = (((.5 \* HCRD) + ((1 / 3) \* HALM)) - ((.5 \* HFECRD) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGCRD = (((.5 \* SCRD) + ((1 / 3) \* SALM)) - ((.5 \* SFECRD) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGCRD = ((.5 \* VCRD) + ((1 / 3) \* VALM)) - ((.5 \* VFECRD) + ((1 / 3) \* VPY))

 GAMMAFEMGCRD = GAMMAGAR \* GAMMACRD

 KDGARCRD = ((TK \* DELTASFEMGCRD) - DELTAHFEMGCRD - (P \* DELTAVFEMGCRD) - (.008314 \* TK \* (LOG(GAMMAFEMGCRD)))) / (.008314 \* TK)

 KDGARCRD = EXP(KDGARCRD)

END IF

IF MODEBT > 0.01 THEN

 REM "CALCULATES A CORRECTED KD(GRT-BT)"

 DELTAHFEMGBT = ((((1 / 3) \* HPHL) + ((1 / 3) \* HALM)) - (((1 / 3) \* HANN) + ((1 / 3) \* HPY))) / 1000

 DELTASFEMGBT = ((((1 / 3) \* SPHL) + ((1 / 3) \* SALM)) - (((1 / 3) \* SANN) + ((1 / 3) \* SPY))) / 1000

 DELTAVFEMGBT = (((1 / 3) \* VPHL) + ((1 / 3) \* VALM)) - (((1 / 3) \* VANN) + ((1 / 3) \* VPY))

 GAMMAGARBT = GAMMABT \* GAMMAGAR

 KDGARBT = ((TK \* DELTASFEMGBT) - DELTAHFEMGBT - (P \* DELTAVFEMGBT) - (.008314 \* TK \* (LOG(GAMMAGARBT)))) / (.008314 \* TK)

 KDGARBT = EXP(KDGARBT)

END IF

REM "QUADRATIC SOLUTION TO CORRECTED MG-RATIOS OF MINERALS"

REM "REQUIRES 10 ITERATIONS (L = 1 TO 10)."

FOR L = 1 TO 10

REM "QUADRATIC SOLUTION TO CORRECTED MG-RATIO OF GARNET AND OPX"

A = MFOPX - (KDGAROPX \* MFOPX)

B = (MFOPX \* KDGAROPX) + MFGAR + (XMGROCK \* KDGAROPX) - XMGROCK - (KDGAROPX \* MGRATIOCRD \* MFCRD) - (KDGAROPX \* MGRATIOBT \* MFBT) + (MFCRD \* MGRATIOCRD) + (MFBT \* MGRATIOBT)

C = (MGRATIOCRD \* MFCRD \* KDGAROPX) + (MGRATIOBT \* MFBT \* KDGAROPX) - (XMGROCK \* KDGAROPX)

MGRATIOOPX = (-B + (((B ^ 2) - (4 \* A \* C)) ^ .5)) / (2 \* A)

MGRATIOGAR = (XMGROCK - (MGRATIOOPX \* MFOPX) - (MGRATIOCRD \* MFCRD) - (MGRATIOBT \* MFBT)) / MFGAR

IF MODEBT > 0.01 THEN

 REM "QUADRATIC SOLUTION TO CORRECTED MG-RATIO OF GARNET AND BIOTITE ""

 A = MFBT - (KDGARBT \* MFBT)

 B = (MFBT \* KDGARBT) + MFGAR + (XMGROCK \* KDGARBT) - XMGROCK - (KDGARBT \* MGRATIOOPX \* MFOPX) - (KDGARBT \* MGRATIOCRD \* MFCRD) + (MFOPX \* MGRATIOOPX) + (MFCRD \* MGRATIOCRD)

 C = (MGRATIOOPX \* MFOPX \* KDGARBT) + (MGRATIOCRD \* MFCRD \* KDGARBT) - (XMGROCK \* KDGARBT)

 MGRATIOBT = (-B + (((B ^ 2) - (4 \* A \* C)) ^ .5)) / (2 \* A)

 MGRATIOGAR = (XMGROCK - (MGRATIOBT \* MFBT) - (MGRATIOOPX \* MFOPX) - (MGRATIOCRD \* MFCRD)) / MFGAR

END IF

IF MODECRD > 0.01 THEN

 REM "QUADRATIC SOLUTION TO CORRECTED MG-RATIO OF GARNET AND CORDIERITE ""

 A = MFCRD - (KDGARCRD \* MFCRD)

 B = (MFCRD \* KDGARCRD) + MFGAR + (XMGROCK \* KDGARCRD) - XMGROCK - (KDGARCRD \* MGRATIOOPX \* MFOPX) - (KDGARCRD \* MGRATIOBT \* MFBT) + (MFOPX \* MGRATIOOPX) + (MFBT \* MGRATIOBT)

 C = (MGRATIOOPX \* MFOPX \* KDGARCRD) + (MGRATIOBT \* MFBT \* KDGARCRD) - (XMGROCK \* KDGARCRD)

 MGRATIOCRD = (-B + (((B ^ 2) - (4 \* A \* C)) ^ .5)) / (2 \* A)

 MGRATIOGAR = (XMGROCK - (MGRATIOCRD \* MFCRD) - (MGRATIOOPX \* MFOPX) - (MGRATIOBT \* MFBT)) / MFGAR

END IF

NEXT L

FERATIOOPX = 1 - MGRATIOOPX

XMGOPX = (MGRATIOOPX) \* ((FE2OPX + MGOPX) / 2)

XFEOPX = (1 - MGRATIOOPX) \* ((FE2OPX + MGOPX) / 2)

XMGGAR = (MGRATIOGAR) \* ((FEGAR + MGGAR) / (FEGAR + MGGAR + CAGAR + MNGAR))

XFEGAR = (1 - MGRATIOGAR) \* ((FEGAR + MGGAR) / (FEGAR + MGGAR + CAGAR + MNGAR))

XMGCRD = MGRATIOCRD \* (XFECRD + XMGCRD)

XFECRD = (1 - MGRATIOCRD) \* (XFECRD + XMGCRD)

XMGBT = MGRATIOBT \* (XFEBT + XMGBT)

XFEBT = (1 - MGRATIOBT) \* (XFEBT + XMGBT)

NEXT I

REM "CALCULATE GRT-OPX FE-MG T TO SEE IF AGREES WITH FINAL FE-AL-OPX T"

 KDGAROPX = (XFEGAR \* XMGOPX) / (XMGGAR \* XFEOPX)

 TGAROPX = (DELTAHFEMGOPX + (P \* DELTAVFEMGOPX)) / (DELTASFEMGOPX - (.008314 \* LOG(KDGAROPX)) - (.008314 \* LOG(GAMMAFEMGOPX)))

 TGAROPX = TGAROPX - 273

IF MODECRD > 0.01 THEN

 REM "CALCULATE GRT-CRD FE-MG T TO SEE IF AGREES WITH FINAL FE-AL-OPX T"

 KDGARCRD = (XFEGAR \* XMGCRD) / (XMGGAR \* XFECRD)

 TGARCRD = (DELTAHFEMGCRD + (P \* DELTAVFEMGCRD)) / (DELTASFEMGCRD - (.008314 \* LOG(KDGARCRD)) - (.008314 \* LOG(GAMMAFEMGCRD)))

 TCGARCRD = TGARCRD - 273

END IF

IF MODEBT > 0.01 THEN

 REM "CALCULATE GRT-BT FE-MG T TO SEE IF AGREES WITH FINAL FE-AL-OPX T"

 KDGARBT = (XFEGAR \* XMGBT) / (XMGGAR \* XFEBT)

 TGARBT = (DELTAHFEMGBT + (P \* DELTAVFEMGBT)) / (DELTASFEMGBT - (.008314 \* LOG(KDGARBT)) - (.008314 \* LOG(GAMMAGARBT)))

 TCGARBT = TGARBT - 273

END IF

REM "CHECK IF RECALCULATED XMGROCK IS THE SAME AS THE INITIAL XMGROCKI"

TEST = (MGRATIOGAR \* MFGAR) + (MGRATIOOPX \* MFOPX) + (MGRATIOCRD \* MFCRD) + (MGRATIOBT \* MFBT)

REM "CALCULATE DIFFERENCES (FINAL - INITIAL)"

DIFFEMGT = TGAROPX - TGAROPXI

DIFFEALT = TC - TFEALI

DIFFEMGP = P - PFEMGGTOPI

DIFFEALP = P - PFEALI

DIFGRTCRDT = TCGARCRD - TCGARCRDI

DIFGRTCRDP = P - PGARCRDI

DIFGRTBTP = P - PGARBTI

DIFGRTBTT = TCGARBT - TCGARBTI

FEMGDIFMFMR = TEST - XMGROCKI

DIFMFMG = MGRATIOGAR - MGRATIOGARI

DIFMFMO = MGRATIOOPX - MGRATIOOPXI

DIFMFMB = MGRATIOBT - MGRATIOBTI

DIFMFMC = MGRATIOCRD - MGRATIOCRDI

REM "PRINT OUT RESULTS"

PRINT #2, ""

PRINT #2, "INITIAL AND CONVERGED P-T ESTIMATES AND MINERAL COMPOSITIONS"

PRINT #2, ""

PRINT #2, " CONVERGED (FINAL) INITIAL DIFFERENCE"

PRINT #2, USING "Fe Al GOPQ#####. C ##.## KB ";TC ;P; USING "#####. C ##.## KB "; TFEALI ; PFEALI; USING "####. C ##.## KB"; DIFFEALT; DIFFEALP

PRINT #2, USING "GrtOpx GOPQ#####. C ##.## KB ";TGAROPX;P; USING "#####. C ##.## KB "; TGAROPXI; PFEMGGTOPI; USING "####. C ##.## KB"; DIFFEMGT; DIFFEMGP

IF MODEBT > 0.01 THEN PRINT #2, USING "GrtBt GOPQ#####. C ##.## KB ";TCGARBT ;P; USING "#####. C ##.## KB "; TCGARBTI ;PGARBTI ; USING "####. C ##.## KB"; DIFGRTBTT ; DIFGRTBTP

IF MODECRD > 0.01 THEN PRINT #2, USING "GrtCrd GOPQ#####. C ##.## KB ";TCGARCRD;P; USING "#####. C ##.## KB "; TCGARCRDI;PGARCRDI; USING "####. C ##.## KB"; DIFGRTCRDT; DIFGRTCRDP

PRINT #2, USING "M/FM rock #.### ";TEST ; USING " #.### "; XMGROCKI ; USING " ##.### "; DIFMFMR

PRINT #2, USING "M/FM Grt #.### ";MGRATIOGAR;USING " #.### "; MGRATIOGARI ; USING " ##.### "; DIFMFMG

PRINT #2, USING "M/FM Opx #.### ";MGRATIOOPX;USING " #.### "; MGRATIOOPXI ; USING " ##.### "; DIFMFMO

IF MODEBT > 0.01 THEN PRINT #2, USING "M/FM Bt #.### ";MGRATIOBT ;USING " #.### "; MGRATIOBTI ; USING " ##.### "; DIFMFMB

IF MODECRD> 0.01 THEN PRINT #2, USING "M/FM Crd #.### ";MGRATIOCRD;USING " #.### "; MGRATIOCRDI ; USING " ##.### "; DIFMFMC

PRINT #2, ""

PRINT ""

INPUT "ANOTHER AL-IN-OPX MODEL (Y/y)"; ANSWER1$

IF ANSWER1$ = "Y" THEN GOTO MODEL

IF ANSWER1$ = "y" THEN GOTO MODEL

PRINT ""

INPUT "ANOTHER SAMPLE (Y/y)"; ANSWER2$

IF ANSWER2$ = "Y" THEN GOTO SAMPLE

IF ANSWER2$ = "y" THEN GOTO SAMPLE

END

REM "SUBROUTINES"

REM "SUBROUTINE ALOPX1"

ALOPX1:

XFEOPX = FE2OPX / 2

XMGOPX = MGOPX / 2

XALM1 = (ALOPX - (2 - SIOPX)) / 2

ALCHOICE$ = "MODEL 1 XAlOpx (1-site Opx) = (Al - (2-Si) )/2"

ALCHOICE2$ = "XFeOpx = Fe2+/2 XMgOpx = Mg/2 "

RETURN

REM "SUBROUTINE ALOPX2"

ALOPX2:

XFEOPX = FE2OPX / 2

XMGOPX = MGOPX / 2

XALM1 = (ALOPX / 2) / 2

ALCHOICE$ = "MODEL 2 XAlOpx (1-site Opx) = (Al/2) / 2"

ALCHOICE2$ = "XFeOpx = Fe2+/2 XMgOpx = Mg/2 "

RETURN

REM "SUBROUTINE ALOPX3"

ALOPX3:

XFEOPX = FE2OPX / (FE2OPX + MGOPX + MNOPX + CAOPX + (ALOPX/2))

XMGOPX = MGOPX / (FE2OPX + MGOPX + MNOPX + CAOPX + (ALOPX/2))

XALM1 = (ALOPX/2) / (FE2OPX + MGOPX + MNOPX + CAOPX + (ALOPX/2))

ALCHOICE$ = "MODEL 3 XAlOpx (1-site Opx) = (Al/2) / sum"

ALCHOICE2$ ="where sum = Fe2+ + Mg + Mn + Ca + (Al/2). XFeOpx = Fe2+/sum"

RETURN

REM "SUBROUTINE ALOPX4"

ALOPX4:

XFEOPX = FE2OPX / 2

XMGOPX = MGOPX / 2

XALM1 = (ALOPX-Fe3OPX-CROPX-(2\*TIOPX)) /4

ALCHOICE$ = "MODEL 4 XAlOpx (1-site Opx) = ((Al - Fe3+ - Cr - (2\*Ti))/2) / 2"

ALCHOICE2$ = "XFeOpx = Fe2+/2 XMgOpx = MgOpx/2 "

RETURN

REM "SUBROUTINE CP"

CP:

REM"CALCULATES ENTHALPIES OF PHASES AT T USING STANDARD STATE ENTHALPIES AND HEAT CAPACITY"

REM"EXPRESSIONS FROM TWQ202B - BA96A.DAT OF BERMAN"

HALM = DATASET(1, 1) + ((DATASET(1, 3) \* (TK - 298.15)) + ((2 \* DATASET(1, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(1, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(1, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HPY = DATASET(2, 1) + ((DATASET(2, 3) \* (TK - 298.15)) + ((2 \* DATASET(2, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(2, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(2, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HGR = DATASET(3, 1) + ((DATASET(3, 3) \* (TK - 298.15)) + ((2 \* DATASET(3, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(3, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(3, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HAN = DATASET(4, 1) + ((DATASET(4, 3) \* (TK - 298.15)) + ((2 \* DATASET(4, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(4, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(4, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HBQ = DATASET(5, 1) + ((DATASET(5, 3) \* (TK - 298.15)) + ((2 \* DATASET(5, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(5, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(5, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HEN = DATASET(6, 1) + ((DATASET(6, 3) \* (TK - 298.15)) + ((2 \* DATASET(6, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(6, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(6, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HFS = DATASET(7, 1) + ((DATASET(7, 3) \* (TK - 298.15)) + ((2 \* DATASET(7, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(7, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(7, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HALOPX = DATASET(8, 1) + ((DATASET(8, 3) \* (TK - 298.15)) + ((2 \* DATASET(8, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(8, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(8, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HPHL = DATASET(9, 1) + ((DATASET(9, 3) \* (TK - 298.15)) + ((2 \* DATASET(9, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(9, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(9, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HANN = DATASET(10, 1) + ((DATASET(10, 3) \* (TK - 298.15)) + ((2 \* DATASET(10, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(10, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(10, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HCRD = DATASET(11, 1) + ((DATASET(11, 3) \* (TK - 298.15)) + ((2 \* DATASET(11, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(11, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(11, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

HFECRD = DATASET(12, 1) + ((DATASET(12, 3) \* (TK - 298.15)) + ((2 \* DATASET(12, 4)) \* ((TK ^ .5) - (298.15 ^ .5))) - (DATASET(12, 5) \* ((TK ^ -1) - (298.15 ^ -1))) - (.5 \* DATASET(12, 6) \* ((TK ^ -2) - (298.15 ^ -2))))

REM"CALCULATES ENTROPIES OF PHASES AT T USING STANDARD STATE ENTROPIES AND HEAT CAPACITY"

REM"EXPRESSIONS FROM TWQ202B - BA96A.DAT OF BERMAN"

SALM = DATASET(1, 2) + ((DATASET(1, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(1, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(1, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(1, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SPY = DATASET(2, 2) + ((DATASET(2, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(2, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(2, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(2, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SGR = DATASET(3, 2) + ((DATASET(3, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(3, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(3, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(3, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SAN = DATASET(4, 2) + ((DATASET(4, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(4, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(4, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(4, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SBQ = DATASET(5, 2) + ((DATASET(5, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(5, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(5, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(5, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SEN = DATASET(6, 2) + ((DATASET(6, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(6, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(6, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(6, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SFS = DATASET(7, 2) + ((DATASET(7, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(7, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(7, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(7, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SALOPX = DATASET(8, 2) + ((DATASET(8, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(8, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(8, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(8, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SPHL = DATASET(9, 2) + ((DATASET(9, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(9, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(9, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(9, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SANN = DATASET(10, 2) + ((DATASET(10, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(10, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(10, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(10, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SCRD = DATASET(11, 2) + ((DATASET(11, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(11, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(11, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(11, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

SFECRD = DATASET(12, 2) + ((DATASET(12, 3) \* ((LOG(TK)) - (LOG(298.15)))) - ((2 \* DATASET(12, 4)) \* ((TK ^ -.5) - (298.15 ^ -.5))) - ((.5 \* DATASET(12, 5)) \* ((TK ^ -2) - (298.15 ^ -2))) - (((1 / 3) \* DATASET(12, 6)) \* ((TK ^ -3) - (298.15 ^ -3))))

RETURN

REM "SUBROUTINE VOLUMEPT"

VOLUMEPT:

REM"CALCULATES VOLUMES OF PHASES AT P AND T USING STANDARD STATE VOLUMES AND EXPANSION"

REM"AND COMPRESSIBILITY EXPRESSIONS FROM TWQ202B - BA96A.DAT OF BERMAN"

VALM = 11.524 \* (1 + (.0000185989054# \* (TK - 298)) + (7.4711E-09 \* ((TK - 298) ^ 2)) + (-.000000570324# \* PBARS) + (4.344E-13 \* (PBARS ^ 2)))

VPY = 11.311 \* (1 + (.0000225186544# \* (TK - 298)) + (3.7044E-09 \* ((TK - 298) ^ 2)) + (-.000000576209# \* PBARS) + (4.42E-13 \* (PBARS ^ 2)))

VGR = 12.538 \* (1 + (.0000189942017# \* (TK - 298)) + (7.9756E-09 \* ((TK - 298) ^ 2)) + (-.0000006539136# \* PBARS) + (1.635E-12 \* (PBARS ^ 2)))

VAN = 10.075 \* (1 + (.0000109181141# \* (TK - 298)) + (4.1985E-09 \* ((TK - 298) ^ 2)) + (-.0000012724268# \* PBARS) + (3.1762E-12 \* (PBARS ^ 2)))

VBQ = 2.37 \* (1 + (0 \* (TK - 298)) + (0 \* ((TK - 298) ^ 2)) + (-.0000012382672# \* PBARS) + (7.0871E-12 \* (PBARS ^ 2)))

VEN = 3.133 \* (1 + (.0000246558172# \* (TK - 298)) + (7.467E-09 \* ((TK - 298) ^ 2)) + (-.0000007493458# \* PBARS) + (4.467E-13 \* (PBARS ^ 2)))

VFS = 3.295 \* (1 + (.0000314064017# \* (TK - 298)) + (8.04E-09 \* ((TK - 298) ^ 2)) + (-.0000009111044# \* PBARS) + (3.034E-13 \* (PBARS ^ 2)))

VALOPX = 3.093 \* (1 + (.0000246558172# \* (TK - 298)) + (7.467E-09 \* ((TK - 298) ^ 2)) + (-.0000007493458# \* PBARS) + (4.467E-13 \* (PBARS ^ 2)))

VPHL = 14.971 \* (1 + (.0000344473262# \* (TK - 298)) + (0 \* ((TK - 298) ^ 2)) + (-.0000016969784# \* PBARS) + (0 \* (PBARS ^ 2)))

VANN = 15.487 \* (1 + (.0000344473262# \* (TK - 298)) + (0 \* ((TK - 298) ^ 2)) + (-.0000016969784# \* PBARS) + (0 \* (PBARS ^ 2)))

VCRD = 23.311 \* (1 + (.0000030028742# \* (TK - 298)) + (1.8017E-09 \* ((TK - 298) ^ 2)) + (-.0000011582515# \* PBARS) + (0 \* (PBARS ^ 2)))

VFECRD = 23.706 \* (1 + (.0000042647431# \* (TK - 298)) + (0 \* ((TK - 298) ^ 2)) + (-.0000016998228# \* PBARS) + (0 \* (PBARS ^ 2)))

RETURN

REM "SUBROUTINE BERMAN"

BERMAN:

REM "THIS SUBROUTINE CALCULATES GARNET ACTIVITIES FOR CA-FE-MG-MN GARNET WITH THE MODEL"

REM "IN TWQ202B - BA96a.SLN OF BERMAN"

X1 = XCAGAR

X2 = XMGGAR

X3 = XFEGAR

X4 = XMNGAR

W112 = 85529! - (TK \* 18.79) + (PBARS \* .21)

W122 = 50874.9 - (TK \* 18.79) + (PBARS \* .02)

W113 = 24025.5 - (TK \* 9.43) + (PBARS \* .17)

W133 = 9876.2 - (TK \* 9.43) + (PBARS \* .09)

W223 = 1307.4 + (PBARS\* .01)

W233 = 2092.4 + (PBARS\* .06)

W123 = 86852.8 - (TK \* 28.22) + (PBARS \* .28)

W124 = 82759.9 - (TK \* 28.79) + (PBARS \* .1)

W134 = 7053.9 + (TK \* 30.01) + (PBARS \* .13)

W234 = 6361! + (TK \* 29.44) + (PBARS \* .04)

W224 = 14558! - (TK \* 10!) + (PBARS \* .04)

W244 = 14558! - (TK \* 10!) + (PBARS \* .04)

W344 = 158! + (TK \* 35.1) + (PBARS \* .04)

W334 = (-19952!) + (TK \* 43.78) + (PBARS \* .04)

TERM1GR = (W112 \* ((2 \* X1 \* X2) - (2 \* (X1 ^ 2) \* X2))) + (W122 \* ((X2 ^ 2) - (2 \* X1 \* (X2 ^ 2))))

TERM2GR = (W113 \* ((2 \* X1 \* X3) - (2 \* (X1 ^ 2) \* X3))) + (W133 \* ((X3 ^ 2) - (2 \* X1 \* (X3 ^ 2))))

TERM3GR = (W114 \* ((2 \* X1 \* X4) - (2 \* (X1 ^ 2) \* X4))) + (W144 \* ((X4 ^ 2) - (2 \* X1 \* (X4 ^ 2))))

TERM4GR = (W223 \* ((-2) \* (X2 ^ 2) \* X3)) + (W233 \* ((-2) \* X2 \* (X3 ^ 2)))

TERM5GR = (W224 \* ((-2) \* (X2 ^ 2) \* X4)) + (W244 \* ((-2) \* X2 \* (X4 ^ 2)))

TERM6GR = (W334 \* ((-2) \* (X3 ^ 2) \* X4)) + (W344 \* ((-2) \* X3 \* (X4 ^ 2)))

TERM7GR = (W123 \* ((X2 \* X3) - (2 \* X1 \* X2 \* X3))) + (W124 \* ((X2 \* X4) - (2 \* X1 \* X2 \* X4)))

TERM8GR = (W134 \* ((X3 \* X4) - (2 \* X1 \* X3 \* X4))) + (W234 \* ((-2) \* X2 \* X3 \* X4))

SUMGR = TERM1GR + TERM2GR + TERM3GR + TERM4GR + TERM5GR + TERM6GR + TERM7GR + TERM8GR

GAMMAGR = EXP(SUMGR / (3 \* 8.314 \* TK))

AGR = ((X1 \* GAMMAGR) ^ 3)

TERM1PY = (W112 \* ((X1 ^ 2) - (2 \* X2 \* (X1 ^ 2)))) + (W122 \* ((2 \* X1 \* X2) - (2 \* (X2 ^ 2) \* X1)))

TERM2PY = (W113 \* ((-2) \* (X1 ^ 2) \* X3)) + (W133 \* ((-2) \* X1 \* (X3 ^ 2)))

TERM3PY = (W114 \* ((-2) \* (X1 ^ 2) \* X4)) + (W144 \* ((-2) \* X1 \* (X4 ^ 2)))

TERM4PY = (W223 \* ((2 \* X2 \* X3) - (2 \* (X2 ^ 2) \* X3))) + (W233 \* ((X3 ^ 2) - (2 \* X2 \* (X3 ^ 2))))

TERM5PY = (W224 \* ((2 \* X2 \* X4) - (2 \* (X2 ^ 2) \* X4))) + (W244 \* ((X4 ^ 2) - (2 \* X2 \* (X4 ^ 2))))

TERM6PY = (W334 \* ((-2) \* (X3 ^ 2) \* X4)) + (W344 \* ((-2) \* X3 \* (X4 ^ 2)))

TERM7PY = (W123 \* ((X1 \* X3) - (2 \* X1 \* X2 \* X3))) + (W124 \* ((X1 \* X4) - (2 \* X1 \* X2 \* X4)))

TERM8PY = (W134 \* ((-2) \* X1 \* X3 \* X4)) + (W234 \* ((X3 \* X4) - (2 \* X2 \* X3 \* X4)))

SUMPY = TERM1PY + TERM2PY + TERM3PY + TERM4PY + TERM5PY + TERM6PY + TERM7PY + TERM8PY

GAMMAPY = EXP(SUMPY / (3 \* 8.314 \* TK))

APY = ((X2 \* GAMMAPY) ^ 3)

TERM1AL = (W112 \* ((-2) \* (X1 ^ 2) \* X2)) + (W122 \* ((-2) \* X1 \* (X2 ^ 2)))

TERM2AL = (W113 \* ((X1 ^ 2) - (2 \* X3 \* (X1 ^ 2)))) + (W133 \* ((2 \* X1 \* X3) - (2 \* (X3 ^ 2) \* X1)))

TERM3AL = (W114 \* ((-2) \* (X1 ^ 2) \* X4)) + (W144 \* ((-2) \* X1 \* (X4 ^ 2)))

TERM4AL = (W223 \* ((X2 ^ 2) - (2 \* X3 \* (X2 ^ 2)))) + (W233 \* ((2 \* X2 \* X3) - (2 \* (X3 ^ 2) \* X2)))

TERM5AL = (W224 \* ((-2) \* (X2 ^ 2) \* X4)) + (W244 \* ((-2) \* X2 \* (X4 ^ 2)))

TERM6AL = (W334 \* ((2 \* X3 \* X4) - (2 \* (X3 ^ 2) \* X4))) + (W344 \* ((X4 ^ 2) - (2 \* X3 \* (X4 ^ 2))))

TERM7AL = (W123 \* ((X1 \* X2) - (2 \* X1 \* X2 \* X3))) + (W124 \* ((-2) \* X1 \* X2 \* X4))

TERM8AL = (W134 \* ((X1 \* X4) - (2 \* X1 \* X3 \* X4))) + (W234 \* ((X2 \* X4) - (2 \* X2 \* X3 \* X4)))

SUMAL = TERM1AL + TERM2AL + TERM3AL + TERM4AL + TERM5AL + TERM6AL + TERM7AL + TERM8AL

GAMMAAL = EXP(SUMAL / (3 \* 8.314 \* TK))

AAL = ((X3 \* GAMMAAL) ^ 3)

GAMMAGAR = GAMMAAL / GAMMAPY

RETURN

REM "SUBROUTINE FUHRMAN"

FUHRMAN:

REM "THIS SUBROUTINE CALCULATES PLAGIOCLASE ACTIVITIES WITH THE MODEL"

REM "IN TWQ202B - BA96a.SLN OF BERMAN. IT IS THE MODEL OF FUHRMAN AND LINDSLEY (1988)"

REM "WITH WORABAN MODIFIED BY BERMAN FOR TWQ202B."

WABOR = 18.81 - (TK \* .0103) + (P \* .39)

WORAB = 27.32 - (TK \* .0103) + (P \* .39)

WABAN = 28.226

WANAB = 8.471

WANOR = 52.468 - (P \* .12)

WORAN = 47.396

WORABAN = 100.0455# - (TK \* .0103) - (P \* .76)

FIRSTTERM = WORAB \* (XAB \* XORT \* (.5 - XAN - (2 \* XAB)))

SECONDTERM = WABOR \* (XAB \* XORT \* (.5 - XAN - (2 \* XORT)))

THIRDTERM = WORAN \* ((2 \* XORT \* XAN \* (1 - XAN)) + (XAB \* XORT \* (.5 - XAN)))

FOURTHTERM = WANOR \* (((XORT ^ 2) \* (1 - (2 \* XAN))) + (XAB \* XORT \* (.5 - XAN)))

FIFTHTERM = WABAN \* ((2 \* XAB \* XAN \* (1 - XAN)) + (XAB \* XORT \* (.5 - XAN)))

SIXTHTERM = WANAB \* (((XAB ^ 2) \* (1 - (2 \* XAN))) + (XAB \* XORT \* (.5 - XAN)))

SEVENTHTERM = WORABAN \* (XORT \* XAB \* (1 - (2 \* XAN)))

AAN = EXP((FIRSTTERM + SECONDTERM + THIRDTERM + FOURTHTERM + FIFTHTERM + SIXTHTERM + SEVENTHTERM) / (.008314 \* TK))

AAN = (XAN \* (((1 + XAN) ^ 2) / 4)) \* AAN

RETURN

REM "SUBROUTINE MCMULLIN"

MCMULLIN:

REM"THIS SUBROUTINE CALCULATES ANNITE AND PHLOGOPITE ACTIVITIES WITH THE MODEL"

REM"OF MCMULLIN (1991). IT IS THUS DIFFERENT FROM THE MODEL IN TWQ202B - BA96a.SLN OF BERMAN."

WMGFE = 0

WMGTI = 58.865

WMGAL = 75

WFETI = 30.921

WFEAL = 63.721

WTIAL = 0

RTGAMMAMGBT = ((XFEBT ^ 2) \* WMGFE) + ((XTIBT ^ 2) \* WMGTI) + ((XALBT ^ 2) \* WMGAL) + (XFEBT \* XTIBT \* (WMGFE + WMGTI - WFETI)) + (XFEBT \* XALBT \* (WMGFE + WMGAL - WFEAL)) + (XTIBT \* XALBT \* (WMGTI + WMGAL - WTIAL))

RTGAMMAFEBT = ((XMGBT ^ 2) \* WMGFE) + ((XTIBT ^ 2) \* WFETI) + ((XALBT ^ 2) \* WFEAL) + (XMGBT \* XTIBT \* (WMGFE + WFETI - WMGTI)) + (XMGBT \* XALBT \* (WMGFE + WFEAL - WMGAL)) + (XTIBT \* XALBT \* (WFETI + WFEAL - WTIAL))

GAMMAMGBT = EXP(RTGAMMAMGBT / (.008314 \* TK))

GAMMAFEBT = EXP(RTGAMMAFEBT / (.008314 \* TK))

GAMMABT = GAMMAMGBT / GAMMAFEBT

RETURN

REM "SUBROUTINE CORDIERITE"

CORDIERITE:

REM"THIS SUBROUTINE CALCULATES MGCRD AND FECRD ACTIVITIES WITH THE MODEL"

REM"IN TWQ202B - BA96a.SLN OF BERMAN"

WCRD = -1754.7

RTGAMMAMGCRD = WCRD \* ((1 - MGRATIOCRD) ^ 2)

RTGAMMAFECRD = WCRD \* (MGRATIOCRD ^ 2)

GAMMAMGCRD = EXP(RTGAMMAMGCRD / (8.314 \* TK))

GAMMAFECRD = EXP(RTGAMMAFECRD / (8.314 \* TK))

GAMMACRD = GAMMAMGCRD / GAMMAFECRD

RETURN

REM "SUBROUTINE ARANOVICH"

ARANOVICH:

REM"THIS SUBROUTINE CALCULATES OPX ACTIVITIES WITH THE MODEL"

REM"IN TWQ202B - BA96a.SLN OF BERMAN. IT IS BASED ON THE MODEL OF ARANOVICH AND BERMAN (1997)"

REM"NOTE THAT THE ALOPX ACTIVITY MODEL INCLUDES A DARKEN CORRECTION OF THE FORM"

REM"RTLN(GAMMA)ALOPX =RTLN(GAMMA)ALOPX + FE/(FE+MG)\*(DH-T\*DS)"

W12 = -4543.8 + (TK \* 3.36)

W23 = -32213.3 - (PBARS \* .69)

W13 = -26944.5 - (PBARS \* .58)

RTGAMMAMGOPX=(W12\*(XFEOPX-(XFEOPX\*XMGOPX)))-(W23\*XFEOPX\*XALM1)+(W13\*(XALM1-(XMGOPX\*XALM1)))

RTGAMMAFEOPX=(W12\*(XMGOPX-(XFEOPX\*XMGOPX)))+(W23\*(XALM1-(XFEOPX\*XALM1)))-(W13\*XMGOPX\*XALM1)

RTGAMMAALOPX=(-1\*(W12\*XFEOPX\*XMGOPX))+(W23\*(XFEOPX-(XFEOPX\*XALM1)))+(W13\*(XMGOPX-(XMGOPX\*XALM1)))+(FERATIOOPX\*(24307!-(TK\*14.404)+(PBARS\*.185)))

GAMMAMGOPX = EXP(RTGAMMAMGOPX / (8.314 \* TK))

GAMMAFEOPX = EXP(RTGAMMAFEOPX / (8.314 \* TK))

GAMMAALOPX = EXP(RTGAMMAALOPX / (8.314 \* TK))

AEN = XMGOPX \* GAMMAMGOPX

AFS = XFEOPX \* GAMMAFEOPX

AALOPX = XALM1 \* GAMMAALOPX

GAMMAOPX = GAMMAMGOPX / GAMMAFEOPX

RETURN

REM "THERMODYNAMIC DATA OF TWQ202B - BA96a.DAT OF BERMAN"

REM " H, S, K0, K1, K2, K3"

REM "ALM, PYROPE, GROSSULAR, ANORTHITE, B-QTZ, EN, FS, AL-OPX, PHL, ANN, CRD, FE-CRD"

DATA -5265317.1,341.5824,621.4269,-3287.931,-15081040,2211865100

DATA -6284733.7,268.8,590.9042,-2826.956,-13320810,1260328500

DATA -6632861,255.15,573.43042,-2039.405,-18887168,2319311872

DATA -4228730,200.1861,439.36938,-3734.149,0,-317023232

DATA -908626.8,44.2068,80.01199,-240.276,-3546684,491568384

DATA -1546037.1,66.18,166.5795,-1200.588,-2270560,279150300

DATA -1192860,96.5587,174.2024,-1392.959,-454390,-37711400

DATA -1631665.9,35.375,119.38,774.808,-6509130,422877600

DATA -6216676.7, 325.9239,610.37988,-2083.781,-21533008,2841040896

DATA -5155234.4,405.01,727.208,-4775.04,-13831900,2119060000

DATA -9161425.7,416.2714,954.3865,-7962.274,-2317258,-370214090

DATA -8429860.2,482.8282,983.479,-8403.659,-1870290,-85683500