

DENSCAL: A PROGRAM FOR CALCULATING DENSITIES OF SILICATE MELTS AND MANTLE MINERALS AS A FUNCTION OF PRESSURE, TEMPERATURE, AND COMPOSITION IN MELTING RANGE

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(Received 20 June 1990; accepted 26 November 1990)

Abstract—A computer program is presented based on a new up-to-date compilation of mineral and melt densities, compressibilities, and thermal expansivities, which can be used to calculate *in-situ* densities of solid assemblages of minerals and basaltic melts. This program is useful for quantitatively assessing buoyancy forces of melts, solids, and solid-liquid mixtures in the upper mantle.

Key Words: Density, Olivine, Orthopyroxene, Clinopyroxene, Garnet, Spinel, Plagioclase, Silicate melt, MORB, BASIC.

INTRODUCTION

The *in-situ* densities of solid mantle mineral assemblages and basalt melts are important for evaluating melt migration by porous flow (McKenzie, 1984). In addition, the style of solid mantle upwelling and melt segregation processes are affected by thermal buoyancy forces, compositional buoyancy forces, and the density relations of melt and solid phases (e.g. Sotin and Parmentier, 1989; Scott and Stevenson, 1989; Phipps-Morgan, 1987; Spiegelman and McKenzie, 1987; Buck and Su, 1989). Usually, a constant value of 0.5 g-cm^{-3} is assumed for the density difference between upper mantle melt and solid residue. In order to determine whether this assumption is correct, and to provide an up-to-date compilation of densities, thermal expansivities, and compressibilities for mantle melts and solid phases, we have examined the available data. These results are reported fully in Niu and Batiza (1991a). The purpose of this paper is to review briefly our methodology and to make available the DENSCAL program. This interactive menu-driven program, written in Microsoft BASIC, make it easy to calculate the *in-situ* densities of mantle minerals and melts as a function of temperature, pressure, and composition.

DENSITY CALCULATION

Silicate melts

Temperature effect on melt density. Among the several existing models for calculating the densities of silicate melts, we use that of Lange and Carmichael (1987) because they used the double-bob

Archimedean method for density measurements. In this model, the molar volume of a multicomponent silicate melt has a linear dependence on melt composition with only one excess volume term because of the interaction of TiO_2 and Na_2O :

$$V(T, 1) = \sum X_i(T, 1) \bar{V}_i(T, 1) + X_{\text{Na}_2\text{O}} X_{\text{TiO}_2} \bar{V}_{\text{Na}_2\text{O-TiO}_2} \quad (1)$$

where V is the molar volume of melt, X_i is the oxide (SiO_2 , TiO_2 , Al_2O_3 , Fe_2O_3 , FeO , MgO , CaO , Na_2O , K_2O) mole fraction in the melt, and \bar{V}_i is the partial molar volume of oxide i at temperature T ($^\circ\text{C}$) and 1 atm pressure which is given by

$$\bar{V}_i(T, 1) = \bar{V}_{i,T_R} + \frac{d\bar{V}_i}{dT} (T - T_R) \quad (2)$$

where \bar{V}_{i,T_R} is the partial molar volume of oxide i at the reference temperature T_R (1400°C), and $d\bar{V}_i/dT$ is the temperature derivative of the partial molar volume. Because no partial molar volume data for MnO is available in this model, we use the thermal expansivity data of Bottinga, Weill, and Richet (1982) to obtain it, that is

$$\bar{V}_{\text{MnO}}(T, 1) = 14.13 * \exp[15.1 * 10^{-5} + (T - T_R)]. \quad (3)$$

Thus, the molar volume of the melt at temperature T is $V(T, 1) = V(T, 1)$ [from Eq. (1)] + $\bar{V}_{\text{MnO}}(T, 1)$ [from Eq. (3)] and the density of the silicate melt is given by

$$\rho(T, 1) = \frac{\text{molecular weight of the melt}}{V(T, 1)}. \quad (4)$$

No data for P_2O_5 is available. Model data of \bar{V}_{i,T_R} and $d\bar{V}_i/dT$ required in Equations (1) and (2) are taken from table 8 of Lange and Carmichael (1987).

Pressure effect on melt density. Of the two existing models for handling the pressure effect on the density of natural silicate melts by Lange and Carmichael (1987) and Herzberg (1987a, b), we use that of Lange and Carmichael (1987), because the predictions of this model agree with the results of recent experiments by Agee and Walker (1988). In this model, the isothermal compressibility (β_T) of a silicate linearly depends on the melt composition:

$$\beta_T = \sum X_i \beta_{i,T} \quad (5)$$

where X_i is the mole fraction of oxide i , and β_i is the isothermal compressibility of the oxide which is given by

$$\beta_{i,T} = \beta_i^0 + d\beta_i^0/dT(T - T_R). \quad (6)$$

Data for $\beta_{i,T}$ and $d\beta_i^0/dT$ are from table 12 of Lange and Carmichael (1987). The compressibility of the melt is related simply to the bulk modulus by

$$K_T = 1/\beta_T. \quad (7)$$

Using these data, the pressure effect on the density of silicate melts is evaluated using the well-known third-order Birch–Murnaghan equation of state:

$$P = \frac{3}{2} K_T [R^{7/3} - R^{5/3}] [1 + \frac{3}{4}(4 - K')(R^{2/3} - 1)] \quad (8)$$

where K' is the pressure derivative of K_T^0 , dK_T^0/dP . For silicate melt, $K' \approx 4$ (Lange and Carmichael, 1987; Herzberg, 1987a, 1987b; Agee and Walker, 1988). $R = V(T, 1)/V(T, P) = \rho(T, P)/\rho(T, 1)$, where $\rho(T, 1)$ is calculated by Equation (4), and the unknown $\rho(T, P)$ is evaluated by successive approximation of the pressure calculated by Equation (8) to that of interest.

Solid phases

The solid mineral phases of interest include olivine, orthopyroxene, clinopyroxene, garnet, spinel and plagioclase. Because these phases are solid solutions, in calculating the densities we treat their end-member components individually. Ideal mixing for these solid solutions is assumed when concerned with the temperature effect, and nonideal mixing is treated when considering the pressure effect.

Temperature effect on solid mineral phases. For lengthy and detailed discussions regarding original data source and the derivation of thermal expansions used in this study, interested readers may refer to Niu and Batiza (1991a). The density of a mineral solid solution at 1 atm pressure and temperature of interest may be calculated by

$$\rho(T, 1) = \sum X_i \rho_i(T, 1) \quad (9)$$

where X_i is the mole fraction of end-member i , and $\rho_i(T, 1)$ is the density of the end-member at 1 atm pressure and the temperature of interest which is given by

$$\rho_i(T, 1) = \rho_{25^\circ C}^0 + d\rho^0/dT(T - 25) \quad (10)$$

or

$$\rho_i(T, 1) = \rho_{25^\circ C}^0 + d\rho^0/dT(T - 25) + d^2\rho^0/dT^2(T - 25)^2 \quad (11)$$

where $\rho_{25^\circ C}^0$ refers to the densities of end-members at 1 atm pressure and 25°C, and $d\rho^0/dT$ and $d^2\rho^0/dT^2$ are the first- and second-order temperature derivatives of end-member densities. Equation (10) applies to the end-members of all the mineral phases except forsterite, fayalite, and anorthite for which we use Equation (11). Data for $\rho_{25^\circ C}^0$, $d\rho^0/dT$, and $d^2\rho^0/dT^2$ are from table 1 of Niu and Batiza (1991a).

Pressure effect on solid mineral phases. Equation (8) the third-order Birch–Murnaghan equation of state, is used to evaluate the pressure effect on the solid mineral phases. In Equation (8), the bulk modulus, K_T , for end members is calculated by

$$K_T = K_{T_0} + dK_{T_0}/dT(T - T_R) \quad (12)$$

where K_{T_0} , dK_{T_0}/dT , the temperature derivative of bulk modulus, and K' , the pressure derivative of bulk modulus, are taken from table 1 of Niu and Batiza (1991a). In working with the bulk modulus of a solid solution, we use the Voigt–Reuss–Hill mixing model rather than ideal mixing, that is, the bulk modulus of a solid solution is given by

$$K_T = (K_V + K_R)/2 \quad (13)$$

where

$$K_V = \sum V_i K_{i,T}, \quad K_R = \left[\sum (V_i/K_{i,T}) \right]^{-2},$$

and V_i and $K_{i,T}$ are molar volume and modulus of end-member i respectively.

DENSAL

The program DENSAL, written in microsoft BASIC (see Appendix), uses the new compilation of thermal expansion and elastic data in Niu and Batiza (1991a) and strictly follows the algorithms discussed here and in Niu and Batiza (1991a). Equations (1)–(4) are employed to calculate densities of silicate melts as a function of temperature and composition, and Equations (5)–(8) are used to evaluate the pressure effect on the densities of melts. Using the data compiled in table 1 of Niu and Batiza (1991a), Equations (9)–(12) are used to calculate the densities of solid phases as a function of temperature and composition by ideal mixing. Equations (12) and (8) are used to evaluate the pressure effect on the

densities of the solid phases. The determination of pressure effect on densities of both silicate melts and solid phases is by Equations (8), the Birch-Murnaghan equation of state, and is performed by successive approximations.

The DENSICAL is highly interactive and self-explanatory. Users may select to calculate the densities of any specific mantle phase assemblages desired. Upon making a selection from a menu, the program will prompt the user to input information, which includes temperature ($^{\circ}\text{C}$), pressure (kbar), and major element oxide concentration in wt% for silicate melt and/or molecular % of end members for each of the solid phases. Input changes can be made conveniently any time. Output can be printed or saved as a user-named file as desired.

A ready-to-run code of DENSICAL in Microsoft BASIC is listed in the Appendix. In order for the program to run on IBM or Macintosh, or any other PCs, the code is written in standard language. Free copies of DENSICAL in both Microsoft BASIC and MacPascal are available on a 3.5" Macintosh diskette with RUNTIME from either of the authors upon request.

AN EXAMPLE

In order to understand quantitatively the compositional buoyancy because of density differences be-

tween melt and residue, we calculated densities of basaltic melts, residue solids, and unmelted mantle in a decompression melting regime as shown in Figure 1 assuming bulk mantle composition of MPY-90 (MORB pyrolite with olivine having Fo_{90} of Falloon and Green, 1987). Figure 1 shows that the adiabatically upwelling mantle begins to melt as it crosses the solidus, and the melting mantle (melt plus residue above solidus) will follow a new adiabat. The compositions of silicate melts and residue solids are calculated using an adiabatic decompression melting model (Niu and Batiza, 1991b). This model assumes that upon melting the melt will separate immediately from the residual mantle and at any time only a small amount of newly produced melt is present at equilibrium with the residue. We are interested here in evaluating the density difference between the finite melt and the residue in equilibrium, that is to evaluate the tendency of the melt to buoyantly escape from the residue. Calculated residual solids are converted to minerals using a modified CIPW normative algorithm, which apportions all Al_2O_3 into plagioclase ($P \leq 9$ kbar) or spinel ($P > 9$ kbar). We calculate the densities along four melting paths as shown in Figure 1 (initial melting at 20, 16, 12, and 8 kbar). Figures 2A and 2B show the densities of instantaneously produced melts and equilibrium residues along these melting paths as a function of the total amount of melt that has been produced and extracted. The thick solid lines represent melting paths, and arrows denote the decompression. The stippled lines numbered on

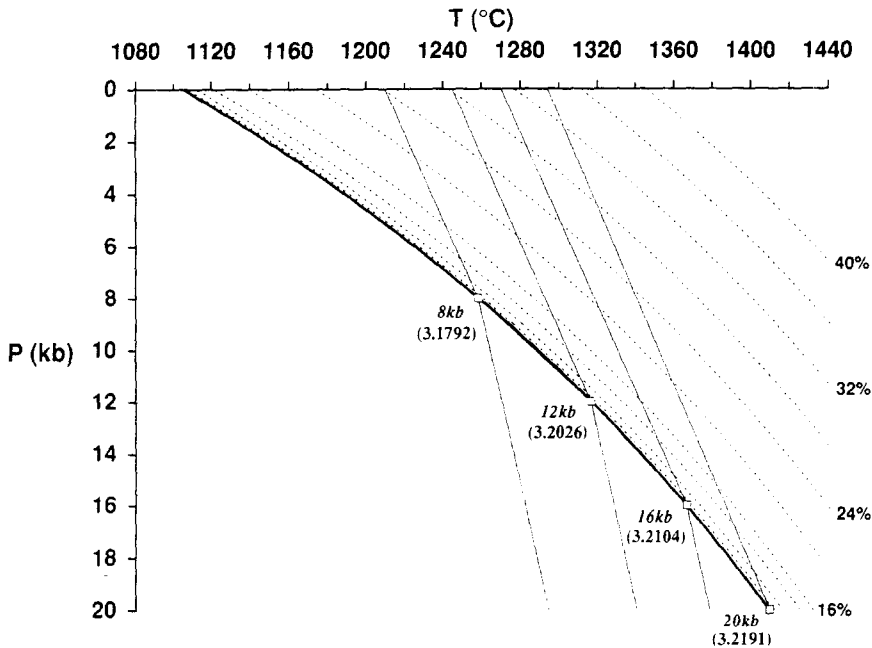


Figure 1. Adiabatic melting paths of upwelling mantle in P - T space. Thick solid lines and thin dashed lines are mantle (MPY-90) solidus and isopleths of extent of partial melting for batch melting case (Niu and Batiza, 1991a, 1991b). Thin solid lines are adiabatic upwelling paths adopted from McKenzie (1984). Pressure values (20, 16, 12, and 8 kbar) indicate initial melting pressures along paths across solidus. Values in parentheses are densities of unmelted mantle at indicated P - T points (\square).

the right are isobars along the decompression melting paths.

The observed decreasing densities for both melts and solids result from both pressure release and compositional changes. Figure 2C shows the density differences ($\rho_{\text{residue}} - \rho_{\text{melt}}$) we calculated. We thus confirm that if melt extraction rate depends strongly on density difference, then the melt extrac-

tion rate increases greatly as depth decreases. However, most recent melting models assume a constant density difference of 0.5 g-cm^{-3} . As seen from Figure 2C, this value is an upper limit, particularly at higher pressures. We expect that our new results may be useful in reassessing compositional and thermal buoyancy for models of mantle flow.

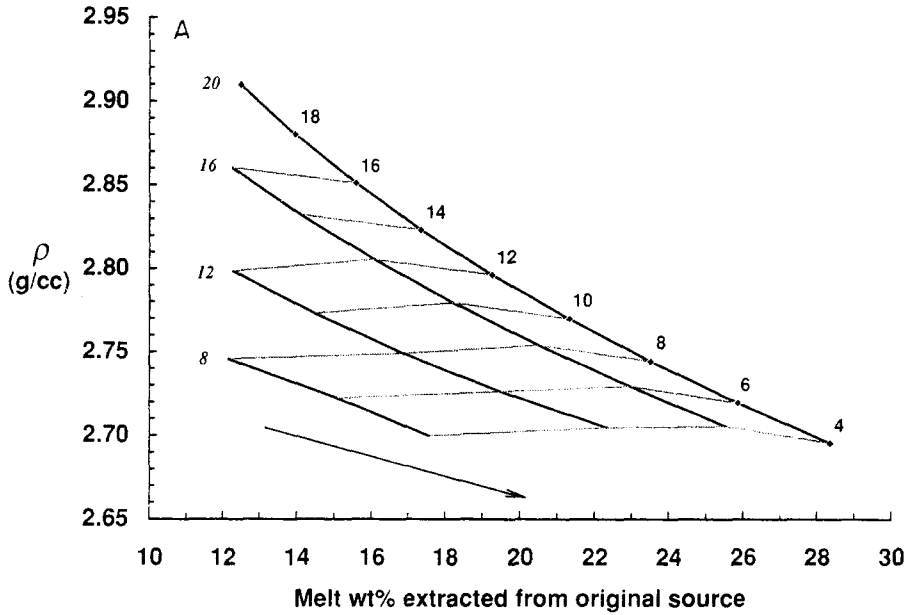


Figure 2A

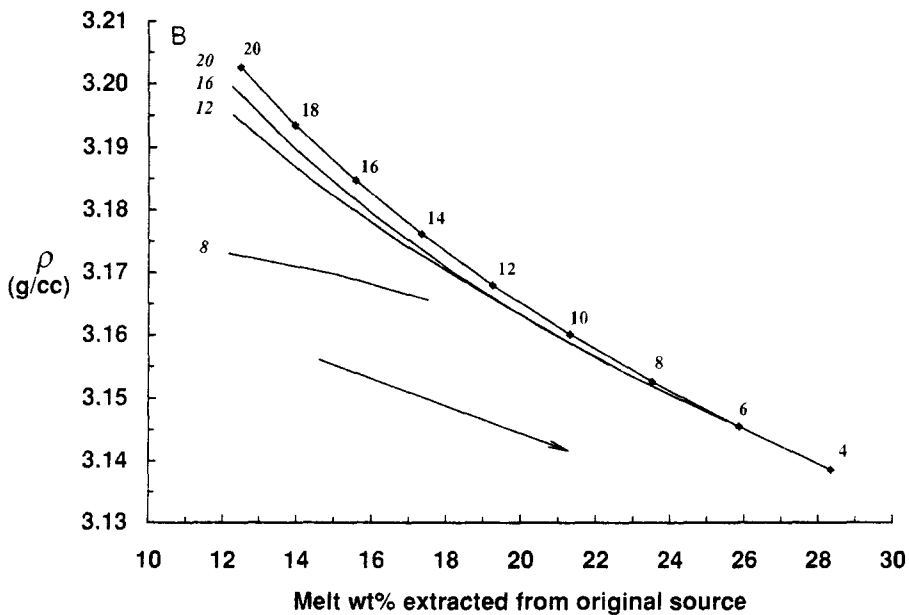


Figure 2B

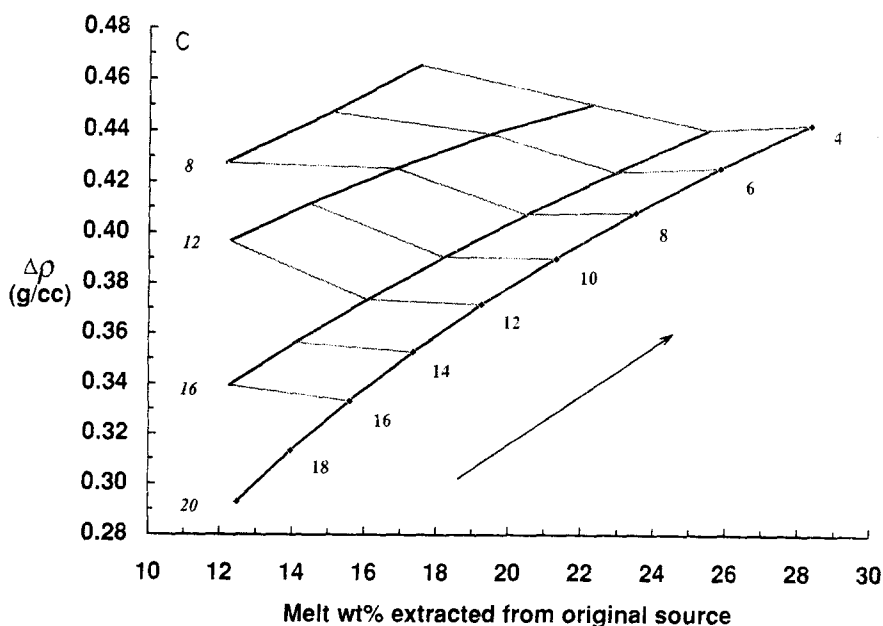


Figure 2C

Figure 2. Calculated densities of silicate melt, residue solids, and density differences between melt and residue for adiabatic decompression melting (Niu and Batiza, 1991b) along melting paths shown in Figure 1. A—Densities of melt as function of wt% melt produced and extracted from residue. Thick solid lines represent melting paths as labeled on left (20, 16, 12, and 8 kb: initial melting pressures). Stippled lines are isobars along these decompression melting paths as labeled on right. Arrow indicates direction of decompression; B—densities of residual solids in equilibrium with melt as function of wt% melt produced and extracted from residue; C—density differences between bulk residue and melt.

Acknowledgments—We acknowledge financial support for this study from the NSF (OCE 89-03296 and OCE-90-00193) and the ONR (N00014-88K-0031) to Dr. Rodey Batiza. Discussion with J. Phipps-Morgan and R. Buck have been helpful.

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APPENDIX

Microsoft BASIC Code for DENSCAL

DENSCAL calculates densities of silicate melts and mantle minerals (olivine, orthopyroxene, clinopyroxene, garnet, spinel, and plagioclase) as a function of TEMPERATURE, PRESSURE, and COMPOSITION in magma generation environment.

First version: 11/15/1989
Second version: 02/23/1990
Final version: 04/22/1990

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OPTION BASE 1

```
DIM OXNS(10),OXW(10),OMW(10),OXMW(10),OXMF(10),PMV0(10),PMV(10)
DIM DVDT(10),BETA(10),DBETADT(10),OXBETA(10),SK(6),SDKDT(6)
DIM SDKDP(6),DST(6),DSPT(6),COMS(6),COM(6),COMW(6),COMV(6)
```

MAINMENU:

```
PRINT TAB(3)"Type one of the numbers (1 - 8) to make choice":PRINT
PRINT TAB(5)"1","DENSITY OF SILICATE MELT"
PRINT TAB(5)"2","DENSITY OF OLIVINE"
PRINT TAB(5)"3","DENSITY OF ORTHOPYROXENE "
PRINT TAB(5)"4","DENSITY OF CLINOPYROXENE "
PRINT TAB(5)"5","DENSITY OF GARNET "
PRINT TAB(5)"6","DENSITY OF SPINEL "
PRINT TAB(5)"7","DENSITY OF PLAGIOCLASE "
PRINT TAB(5)"8","QUIT":PRINT
INPUT "What is your choice":CHOICE
ON CHOICE GOTO MELT,OLIVINE,OPX,CPX,GNT,SPL,PLAG,QUIT
```

MELT:

```
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
RESTORE MELT
FOR I=1 TO 10:READ OXNS(I):NEXT
DATA SiO2,TiO2,Al2O3,Fe2O3,FeO,MnO,MgO,CaO,Na2O,K2O
FOR I=1 TO 10:READ OMW(I):NEXT
DATA 60.0843,79.8988,101.9613,159.6922,71.8464,70.9374,40.32,56.08,61.98,94.2
FOR I=1 TO 10:READ PMV0(I):NEXT
DATA 26.90,23.16,37.11,42.13,13.65,14.13,11.45,16.57,28.78,45.84
FOR I=1 TO 10:READ DVDT(I):NEXT
DATA .0,.00724,.00262,.00909,.00292,.0,.00262,.00292,.00741,.01191
FOR I = 1 TO 10:READ BETA(I):NEXT
DATA 6.93,9.88,5.04,.0,4.28,.0,1.79,0.68,8.35,22.66
FOR I = 1 TO 10:READ DBETADT(I):NEXT
DATA .0,-.5,-13,.0,4,.0,14,3,11,25
NEWSAMPLE:
PRINT:INPUT "Sample Name";SNS
PRINT "Input Oxides wt% of sample"
FOR I=1 TO 10:PRINT OXNS(I);" ";:INPUT OXW(I):OXMW(I)=OXW(I)/OMW(I):NEXT
SUMOFMOL=0:
FOR I=1 TO 10:SUMOFMOL=SUMOFMOL+OXMW(I):NEXT
FOR I=1 TO 10:OXMF(I)=OXMW(I)/SUMOFMOL:NEXT
MOLWTLIQ=0
FOR I=1 TO 10:MOLWTLIQ=MOLWTLIQ+OXMF(I)*OMW(I):NEXT
LPRINT TAB(5)" Melt Sample: ";SNS
LPRINT TAB(5)"-----"
MELTPT:
INPUT "Temperature (°C)":T:INPUT "Pressure (KB)":P
REM MELT DENSITY AT ATMOSPHERIC PRESSURE
FOR I=1 TO 10:PMV(I)=PMV0(I)+DVDT(I)*(T-1400):NEXT
PMV(6)=14.13*EXP(15.1*10^-5*(T-1400))
VLIQ=0
FOR I=1 TO 10:VLIQ=VLIQ+PMV(I)*OXMF(I):NEXT
VLIQ=VLIQ+OXMF(2)*OXMF(9)*20.28
LQDT=MOLWTLIQ/VLIQ:
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```

FOR I=1 TO 10:OXBETA(I)=BETA(I)*10^(-3)+DBETADT(I)*10^(-6)*(T-1400):NEXT
FOR I=1 TO 10:OXBETA(I)=OXBETA(I)*OXMF(I):NEXT
SUMBETA=0
FOR I=1 TO 10:SUMBETA=SUMBETA+OXBETA(I):NEXT
LQMUDULUS=1/SUMBETA
LQDTP=LQDT:MDD=.5
TRYLQ1:
LQDTP=LQDTP+MDD
TRYLQ2:
BM1=BM
BM=1.5*LQMUDULUS*((LQDTP/LQDT)^(7/3)-(LQDTP/LQDT)^(5/3))
IF BM<P AND BM>BM1 THEN GOTO TRYLQ1
IF BM<P AND BM<BM1 THEN MDD=MDD/2:GOTO TRYLQ1
IF BM>P AND BM>BM1 THEN MDD=MDD/2:LQDTP=LQDTP-MDD:GOTO TRYLQ2
IF BM>P AND BM<BM1 THEN LQDTP=LQDTP-MDD: GOTO TRYLQ2
DST=LQDT:DSPT=LQDTP
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO MELTPT
INPUT "Do you want a change of Melt composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO NEWSAMPLE
GOTO MAINMENU

OLIVINE:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SNS
INPUT "Fo%=";FO:FO=FO/100
LPRINT TAB(5)" Olivine Sample: ";SNS
LPRINT TAB(5)"-----"
LPRINT TAB(5)"Fo = ";FO
OLPT:
N=2
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE OLIVINE
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 1271,-0.236,5.39,140.708,1368,-0.268,5.2,203.778
DST(1)=3.225-9.1526*10^(-5)*(T-25)-3.1618*10^(-8)*(T-25)^2
DST(2)=4.4-1.2124*10^(-4)*(T-25)-2.2511*10^(-8)*(T-25)^2
DST=DST(1)*FO+DST(2)*(1-FO)
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO OLPT
INPUT "Do you want a change of Olivine composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO OLIVINE
GOTO MAINMENU

OPX:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SNS
INPUT "En%=";EN:EN=EN/100
N=2
LPRINT TAB(5)" Orthopyroxene Sample: ";SNS
LPRINT TAB(5)"-----"
LPRINT TAB(5)"En = ";EN
OPXPT:
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE OPX
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 1070,-.27,5,200.792,1010,-.3,5,263.862
DST(1)=3.194-9.281*10^(-5)*(T-25):DST(2)=3.998-11.62*10^(-5)*(T-25)
DST=DST(1)*EN+DST(2)*(1-EN)
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO OPXPT
INPUT "Do you want a change of OPX composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO OPX
GOTO MAINMENU

CPX:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SNS
N=6
RESTORE CPX
FOR I=1 TO N:READ COMS(I):NEXT

```

```

DATA CEn,CFs,Di,Hd,Jd,Ac
PRINT "Input % of the following CPX components:"
FOR I=1 TO N: PRINT COM$(I);INPUT COM(I):COM(I)=COM(I)/100:NEXT
LPRINT TAB(5)" Clinopyroxene Sample: ";SN$
LPRINT TAB(5)"-----"
LPRINT TAB(5)"Components: "; "CEn=";COM(1); "CFs=";COM(2);
";Di=";COM(3); "Hd=";COM(4); "Jd=";COM(5); "Ac=";COM(6)

CPXPT:
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE CPXPT
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 1070,-.27,5,200,792,1010,-.3,5,263,862,1130,-.2,4,5,216,56
DATA 1200,-.2,4,5,248,095,1430,-.2,4,5,202,14,1060,-.2,4,5,284,968
DST(1)=3.191-9.272*10^(-5)*(T-25):DST(2)=4.005-11.64*10^(-5)*(T-25)
DST(3)=3.277-2.108*10^(-5)*(T-25):DST(4)=3.632-2.337*10^(-5)*(T-25)
DST(5)=3.347-8.796*10^(-5)*(T-25):DST(6)=3.576-8.796*10^(-5)*(T-25)
DST=0
FOR I=1 TO N:DST=DST+DST(I)*COM(I):NEXT
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO CPXPT
INPUT "Do you want a change of CPX composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO CPX
GOTO MAINMENU

GNT:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SN$
N=6
RESTORE GNT
FOR I=1 TO N:READ COM$(I):NEXT
DATA Pyr,Alm,Gro,Spe,And,Uvr
PRINT "Input % of the following garnet components:"
FOR I=1 TO N: PRINT COM$(I);INPUT COM(I):COM(I)=COM(I)/100:NEXT
LPRINT TAB(5)" Garnet Sample: ";SN$
LPRINT TAB(5)"-----"
LPRINT TAB(5)"Components: "; "Pyr=";COM(1); "Alm=";COM(2);
";Gro=";COM(3); "Spe=";COM(4); "And=";COM(5); "Uvr=";COM(6)

GNTPT:
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE GNTPT
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 1750,-.21,5,45,403,15,1779,-.201,5,43,497,755,1700,-.2,4,25,450,454
DATA 1742,-.2,4,59,495,028,1570,-.2,5,508,185,1620,-.2,5,500,483
DST(1)=3.557-9.332*10^(-5)*(T-25):DST(2)=4.318-11.044*10^(-5)*(T-25)
DST(3)=3.595-8.319*10^(-5)*(T-25):DST(4)=4.19-11.351*10^(-5)*(T-25)
DST(5)=3.86-9.406*10^(-5)*(T-25):DST(6)=3.848-9.378*10^(-5)*(T-25)
DST=0
FOR I=1 TO N:DST=DST+DST(I)*COM(I):NEXT
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO GNTPT
INPUT "Do you want a change of garnet composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO GNT
GOTO MAINMENU

SPL:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SN$
N=4
RESTORE SPL
FOR I=1 TO N:READ COM$(I):NEXT
DATA Spl,Her,Chr,Mgt
PRINT "Input % of the following spinel components:"
FOR I=1 TO N: PRINT COM$(I);INPUT COM(I):COM(I)=COM(I)/100:NEXT
LPRINT TAB(5)" Spinel Sample: ";SN$
LPRINT TAB(5)"-----"
LPRINT TAB(5)"Components: "; "Spl=";COM(1); "Her=";COM(2);
";Chr=";COM(3); "Mgt=";COM(4)

SPLPT:
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE SPLPT
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 1940,-.22,4,142,273,2103,-.2,4,173,808
DATA 1830,-.2,4,223,8366,1860,-.2,4,231,539

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DST(1)=3.583-9.513*10^(-5)*(T-25):DST(2)=4.265-10.423*10^(-5)*(T-25)
DST(3)=5.086-8.907*10^(-5)*(T-25):DST(4)=5.2-21.89*10^(-5)*(T-25)
DST=0
FOR I=1 TO N:DST=DST+DST(I)*COM(I):NEXT
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO SPLPT
INPUT "Do you want a change of spinel composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO SPL
GOTO MAINMENU

PLAG:
CLS
CALL TEXTFONT(0):CALL TEXTSIZE(12):LOCATE 5,5
PRINT:INPUT "Sample Name";SN$
INPUT "An%=";AN:AN=AN/100
N=2
LPRINT TAB(5)" Plagioclase Sample: ";SN$
LPRINT TAB(5)"-----"
LPRINT TAB(5) "An = ";AN
PLAGPT:
INPUT "Temperature (°C)";T:INPUT "Pressure (Kbar)";P
RESTORE PLAG
FOR I=1 TO N:READ SK(I),SDKDT(I),SDKDP(I),COMW(I):NEXT
DATA 699.3,-.2,4,262.223,943.4,-.2,4,278.209
DST(1)=2.611-3.3415*10^(-5)*(T-25)-7.5322*10^(-8)*(T-25)^2
DST(2)=2.762-1.6329*10^(-5)*(T-25)
DST=DST(1)*(1-AN)+DST(2)*AN
GOSUB BCHMNAGAN
GOSUB PRINTER
INPUT "Do you want a change of pressure and temperature (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO PLAGPT
INPUT "Do you want a change of PLAG composition? (Y/N)";Yes$
IF Yes$="Y" OR Yes$="y" THEN GOTO PLAG
GOTO MAINMENU
QUIT:
END

BCHMNAGAN:
FOR I=1 TO N:SK(I)=SK(I)+SDKDT(I)*(T-25):COMV(I)=COMW(I)/DST(I):NEXT
TMV=0:KV=0:KR0=0
FOR I=1 TO N:TMV=TMV+COMV(I):NEXT:
FOR I=1 TO
N:COMV(I)=COMV(I)/TMV:KV=KV+COMV(I)*SK(I):KR0=KR0+COMV(I)/SK(I):NEXT
KR=1/KR0:KT=(KV+KR)/2
PRINT
DSPT=DST:SDD=.5
TRY1:
DSPT=DSPT+SDD
TRY2:
CP1=CP
CP=1.5*KT*((DSPT/DST)^(7/3)-(DSPT/DST)^(5/3))*(1-.75*(4-SDKDP)*((DSPT/DST)^(2/3)-1))
IF CP<P AND CP>CP1 THEN GOTO TRY1
IF CP<P AND CP<CP1 THEN SDD=SDD/2:GOTO TRY1
IF CP>P AND CP>CP1 THEN SDD=SDD/2:DSPT=DSPT-SDD:GOTO TRY2
IF CP>P AND CP<CP1 THEN DSPT=DSPT-SDD: GOTO TRY2
RETURN

PRINTER:
LPRINT TAB(5)"Temperature:      ";T;"°C"
LPRINT TAB(5)"Pressure:          ";P;"Kbar"
LPRINT TAB(5)"Density at ";1;" bar:      ";USING "#.#### g/cc";DST
LPRINT TAB(5)"Density at ";P;" Kb:      ";USING "#.#### g/cc";DSPT
PRINT
RETURN

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