Senior Thesis

A ESTIMATION OF THE PHYSICAL PARAMETERS OF MAGMA CRYSTALLIZATION FOR SANTORINI LAVA USING THERMODYNAMIC METHODS

Presented in Partial Fulfillment of the Requirements for the Degree of Bachelor of Science in the Department of Geological Sciences

> by Todd M. Small The Ohio State University 1996

> > Approved by:

artor

Dr. Michael Barton, Advisor Department of Geological Sciences

Introduction

Accurate procedures now exist that can estimate the pressure and temperature at which magmas crystallize. Knowing these conditions are important for a number of reasons. First, the path of magma evolution can be determined by knowing the pressure and temperature. Furthermore, accurate calculation of pressure and temperature of magma crystallization can give important insight into the depth of magma crystallization at or below the Earth's crust. Finally, knowledge of pressure and temperature of magmas is necessary in order to calculate assorted physical properties of magmas, which in turn, are indispensible for modelling of eruptions and magma flow.

Typically, pressure and temperature of magma crystalization can be determined through experiments. However, predicting the pressure and temperature parameters can also be determined by the use of thermodynamic calculations. There are advantages to this method. Thermodynamic calculations are relatively fast and inexpensive when compared with experiments. Furthermore, when compared to the laborious methods involved in experimental techniques, thermodynamic calculations provide an easy alternative to finding the pressure and temperature parameters of magma crystallization. Finally, thermodynamic calculations are faster than experimentation methods. The scope of this thesis is concerned with the theory and application of these thermodynamic principles and how they relate to a sample basalt from the Santorini volcano located in the Hellenic arc, Greece.

Objectives

The sample basalt that was analyzed for this thesis, originated from a volcanic center on Santorini known as, Micro Profitas Ilias. This is one of four volcanic centers on Santorini that has been studied intensively. Earlier findings have determined that these centers have erupted at different times in Santorini's history, as well as being geochemically distinct from one another (Huijismans and Barton, 1989). To determine whether the sample studied (hereafter, to be referred as slide 138) evolved under the same physical conditions and depth as the other samples taken from different Santorini volcanic centers, methods employing thermodynamic techniques were utilized. These techniques for calculating crystallization conditions are based on chemical compositions of the basalts analyzed. Basalts typically contain phenocrysts with the following components; clinopyroxene (cpx), olivene (ol) and plagioclase (plag). From these chemical components, equilibrium equations can be established. By deriving these equations and then plotting them graphically against each other, the resulting intersection will provide the pressure and temperature of crystallization of that given basalt. The five equilibrium used are as follows:

CaTs+SiO₂=Anorthite

Monticellite+SiO₂=Diopside Forsterite+SiO₂=Clinoenstatite Jadeite+SiO₂=Albite

(CaTs= the Ca-Tschermak's component of clinopyroxene.)

Applying these equations to the other volcanos studied (Patmos, Greece) crystallization temperatures ranged from 1173 to 920° C. Also pressures were determined to range from 2 to 4 kilobars (Barton and Wyers 1991) By interpreting these results, an estimated depth of the magma chambers for these volcanic centers has been determined to range from approximately 6 to 9 kilometers depth. Earlier research of lavas from the Micro Profitas Ilias volcanic center, has shown them to contain Bronzite. Bronzite is pyroxene phenocrysts with cores containing high amounts of aluminum. The high aluminum content in these magmas has been found to be the result of the magma crystallizing in a high pressure environment (Huijsmans and Barton, 1989). Initial analysis of slide 138 has produced results indicating aluminum-rich pyroxene cores. Research performed on other Santorini basalts utilizing the thermodynamic techniques described above, have revealed pressure and temperature of crystallization to be in the range of 2 to 3 kilobars pressure and temperature ranging from 1020-1050°c respectively. These values are consistent with data from earlier measurements as stated above (Barton, unpublished). Variables for silica in a melt are included in each of the above equilibrium. At this time, there is no known method of calculating the variable composition, or activity of silica. Therefore, three or more of the equilibrium must be

must be solved simultaneously for pressure, temperature, and silica activity in order to get accurate results for the conditions of crystallization of a magma. It should be noted however, that the thermodynamic techniques that have been applied towards the Santorini basalts, can also be applied towards any igneous sample.

Electron Microprobe Methodology

The first step in determining the pressures and temperatures of magma crystallization, is to obtain the exact chemical content. This is achieved through the use of an electron microprobe. The chemical composition of slide138 was determined in this way. The microprobe used was a Cameca SX-50 microprobe equipped with four wavelength -dispersive and one energy dispersive spectrometers. The analysis that comprises the data in this thesis was performed on August 1, 1995. Approximately, 20 hours were spent working with the microprobe, when considering calibrations necessary for accurate analysis. Analysis focused on obtaining data from pyroxene phenocrysts in the basalt sample (slide 138). One technique employed to maximize the value of the data, was to analyze both the edges and the cores of pyroxene phenocrysts, in order to differentiate compositional differences within each phenocryst being formed under different physical conditions than the rims. This may be due to the fact that the cores of the

phenocrysts were crystallized at different depths than the rims. During analysis, the electron beam was set at one micron and an accelerating voltage of 15kV. Current for the probe was set to 20nA. Earlier work on this basalt sample by Dr. Barton, included analysis for plagioclase, pyroxene, magnetite, as well as, olivene analysis. The pyroxene data obtained from this basalt was subsequently added to the earlier pyroxene data. Figure 1., below, is a spreadsheet data set showing the combined pyroxene data.

Figure 1.

	Na	Fe	Ti	Si	Ca	Mn	Al	Ni	Mg	Cr	Sum	Mg#
SI138 GR1 CORE	0.0203	0.4057	0.011758	1.919551	0.78843	0.018793	0.059292	0	0.825372	0	4.049195	0.67045
SI138 GR1 CORE	0.020159	0.426867	0.017034	1.87245	0.807508	0.018345	0.083559	0	0.832874	0	4.078806	0.661147
SI138 GR1 RIM	0.016639	0.396121	0.014925	1.872388	0.732504	0.012606	0.07523	0.000807	0.962171	0.000403	4.083795	0.708368
SI138 GR2 CORE O	0.005648	0.777351	0.011397	1.884513	0.210331	0.023602	0.041051	0.001513	1.130981	0.000101	4.086489	0.592654
RIM OF LAST WE	0.022324	0.475748	0.024134	1.876032	0.705397	0.014481	0.112325	0	0.824392	0.000201	4.055035	0.634079
SI 138 PHENO CO	0.022579	0.43727	0.019757	1.860755	0.746381	0.013306	0.10211	0	0.877567	0	4.079723	0.667434
SI138 RIM OF ABO	0.033273	0.300468	0.019359	1.833147	0.82007	0.00857	0.171609	0	0.891829	0.001714	4.08004	0.747992
SI138 RIM OF SAM	0.016441	0.319345	0.016744	1.851001	0.803749	0.012003	0.112265	0.000202	0.952593	0.000706	4.085049	0.74893
MEGA CORE SA	0.026562	0.427501	0.015351	1.844818	0.745282	0.013735	0.119979	0	0.899846	0.002121	4.095294	0.677928
AS ABOVE NEW S	0.026712	0 407228	0.019454	1.857213	0.76018	0.012398	0.134959	0.001008	0.850042	0.004133	4.073337	0.676101
ST138 PYR1 core	0.101	0.262	0.014	1.802	0.717	0.009	0.45	0	0.655	0.001	4.009	0.7144
ST138 PYR2 core	0.057	0.39	0.022	1.86	0.705	0.013	0.2	٥	0.801	0.001	4.047	0.6726
ST138 PYR2 rim	0.05	0.382	0.021	1.877	0.697	0.012	0.197	0	0.786	0	4.033	0.6729
ST138 PYR4 core	0.025	0.417	0.02	1.837	0.759	0.013	0.122	0	0.899	0.002	4.094	0.6831
ST138 PYR5 lg.edge	0.083	0.64	0.022	1.947	0.572	0.01B	0.046	0	0.72	0.001	4.049	0.5291
ST138 PYR5 lg. core	0.043	0.404	0.018	1.846	0.739	0.012	0.156	0	0.861	0.001	4.079	0.6808
ST138 PYR6 core	0.024	0.426	0.02	1.835	0.777	0.012	0.097	0	0.915	0.001	4.108	0.6821
ST138 PYR 13 core	0.027	0.541	0.018	2.002	0.406	0.02	0.143	0	0.765	0	3.923	0.5858

Thermodynamic Background

.

After obtaining probe analyses, the data is processed in a number of computer programs

that calculate the pressure and temperature of magma crystallization. In order to get this result, the computer programs must first calculate the chemical potentials of the separate chemical equilibrium shown previously.

The equation for the chemical potential in an ideal phase is

$$\mu_i = \mu^0 + RTlnX_i$$

In this equation, R= the gas constant, μ° represents the chemical potential of a pure end member I found at standard pressure and temperature. X_i represents the mole fraction, which in this study is the silica activity. The chemical potential is defined as the energy in one mole of substance available for a reaction, this is also known as Gibb's free energy, G. The equation for the change in Gibb's free energy at equilibrium is:

$$\Delta G_{reaction} = 0 = X_c \mu_c + X_d \mu_d - X_a \mu_a - X_b \mu_b$$

By reworking this equation, the combined mole fractions in this equation can be given a new value known as the equilibrium constant, or K. The equation can then be written in the form:

$$RlnK = -(\Sigma X_i \mu_i)/T$$

The change in Gibb's free energy can also be expressed as

$$\Delta G_{reaction} = \Sigma G_{products} - \Sigma G_{reactants}$$

To calculate the standard state Gibb's free energy, G^o , which refers to the Gibb's free energy for a pure phase, A, this expression is used (Barton, unpublished).

$$G_A^{o} = H_A^{o} = -TS_A^{o} + (P-I)V_A^{o}$$

In this equation, H=enthalpy, V=volume and S = entropy. However, this equation only

deals with pure phases, which means a temperature of 298K and at a pressure of 0.001 The equation in this form, is unsuitable for calculating chemical potentials of igneous rocks which crystallize at much higher pressures and temperatures. Therefore, corrections have to be made in order to get free energy equations that work for the basalts analyzed. The following equations correct for elevated temperature and pressure values and their effects on entropy, volume and enthalpy respectively.

$$S^{P,T} S^{P,r} f_{T_{a}} \int_{T_{r}}^{T} (C_{p}/T) dT - \int_{P_{r}}^{P} (\partial V/\partial \Gamma)_{P} dP$$

$$V^{P,T}/V^{Pr,Tr} = I + v_1 (P - P_r) + v_2 (P - P_r)^2 + v_3 (T - T_r) + v_4 (T - T_r)^2$$

$$\Delta_a H^{P,T} + \Delta_f H^{P,T} + \int_{Tr}^{T} C_p dT + \int_{Pr}^{P} \{V^{pr,Tr} - T(\partial V / \partial T)_p\} dP$$

Where C_p is the heat capacity (Berman, 1991). The mole fractions in the equations refer to the SiO2 liquid melt. Therefore, standard-state variables for pure liquid components are calculated. These calculations for standard state entropy and enthalpy for a liquid component are respectively;:

$$S^{o}_{liq}(T_{r}) = S^{o}_{THIRDLAW298} + f_{298}^{Tflus}(C^{o}_{p-sol}/T) dT + \Delta S^{o}_{flus}(T_{flus}) + f_{Tflus}^{T}(C_{Pliq}^{o}/T) dT$$

$$H^{o}_{lig}(T_{r)} = \Delta_{f}H^{o}_{SOL298} + \int_{298}^{T_{fus}}C^{o}_{PsoldT} + \Delta H^{o}_{fus}(T_{fus}) + \int^{T}_{tfus}C^{o}_{Plig}dT$$

With the last two terms in the equation representing heat of fusion and liquid heat capacity respectively (Lange and Carmichael, 1990).

As stated previously, the silica activities cannot be determined on their own. This is due to the fact that the amount of silica cannot be precisely determined. This is because repulsive and attractive forces amongst the components in a solution can change the chemical behavior of the components (Barton, unpublished). The equation for component activity is:

$$a_i = x_i \gamma_i$$

The variable γ , is the activity coefficient and is used to represent the forces that alter the chemical affinities for the given component in the equation. (Barton, unpublished). This can then be combined to the Gibb's free energy equation for a solution. By introducing this variable, which is non-ideal, the equation changes form to:

$$G_{solution} = \Sigma_i x_i / \mu_i^o + RTln x_i + RTln \gamma_i /$$

The first two terms in this equation represent the ideal components, however, the third term introduces the non-ideal component to the equation. This is known as the **excess Gibb's free energy.**

Results and Discussion

The concepts in this thesis were put to practical use after a microprobe analysis was completed on a Santorini basalt (slide 138, discussed previously). Pyroxenes were the focus of this study. The pyroxene data was subsequently input into a computer program designed by Dr. Barton that calculated the thermodynamic equations for each of the pyroxene analyses. These results were then input into a data file (Quattro Pro spreadsheet). This new data set was then input into another series of programs that calculated silica activities of the pyroxenes, over a range of pressures and temperatures. This data was then combined with feldspar data from the same sample. As was stated previously, at least three reactions need to be determined simultaneously in order to compensate for the silica activity present in each of the reactions. The specific reactions that were utilized for the data present in this thesis were as follows:

pyroxenes- fosterite+melt=clinoenstatite

monticellite+melt=diopside

feldspars- CaTs+melt=anorthite

These reactions were then plotted graphically over a range of silica activities and temperatures. These reactions where plotted against each other in order to find intersection points between values at the same pressures. These intersection points from each of the two sets of reactions were then plotted against each other. The intersection point of these two data sets is a graphical representation of the temperature, silica activity and pressure parameters of magma crystallization.

Conclusion

The following plots (figures 2 through 4) pertain to magma crystallization parameters of

slide 138., a sample of a basalt from the Micro Profitas Ilias volcanic center on Santorini.

The results derived from the plots indicate a temperature and pressure of magma crystallization for this basalt to be 1028° C. and approximately 7- 8 k bars respectively.. If this data is accurate, This implies magma crystallization occurred at a depth of approximately 21 to 24 kilometers. Basalts from other volcanic centers on Santorini, have given evidence of having crystallized at a depth of 6 to 9 kilometers (MacCracken, 1993). The crust beneath Santorini is approximately 21 - 24 kilometers thick. The disparity between the depth of crystallization of Micro Profitas Ilias basalts compared to the magma crystallization depth of other Santorini basalts, could be attributed to the presence of a magma chamber located at the base of the crust, as well as, the presence of a shallower magma chamber within the crust which appears to be the source of the other Santorini basalts. This would indicate two stages of magma evolution. More microprobe analyses on the Santorini basalts are needed in order to verify or refute this conclusion.



Figure 2: Plot showing reaction ranges for slide 138 (Micro Profitas Ilias, Santorini)



Figure 3: Plot indicating reaction ranges and intersection points for slide138





Acknowledgments

I would like to thank Dr. Barton for his instruction and being my advisor for this thesis. I would also like to thank Michael Comerford for his expertise and patience while instructing me on the use of the microprobe.

Appendix

The following pages contain the data sheets for the preceding graphs. Included are chemical reactions and silica activity values over a range of pressures and temperatures.

ENTHALPY AND ENTROPY OF FUSION CALCULATED FROM DATA OF RICHET ET AL(GCA, 1982), COMBINED WITH DATA FOR B-QTZ FROM BERMAN (1988). VOLUMES OF FO, FA, CEN, FS MO, DI, AND EXPANSION AND COMPRESSION TERMS FROM BERMAN, J PET, 1988. VOLUME OF SILICA MELT, COMPRESSIBILITY AND EXPANSION CALCULATED FROM DATA OF KRESS AND CARMICHAEL, CMP, 1991.

ACTIVITY OF FO, FA, MO FROM DAVIDSON AND LINDSLEY, AM MIN, 1989. ACTIVITY OF CEN, FS, DI FROM DAVIDSON AND LINDSLEY, AM MIN, 1989.

CA ASSIGNED ONLY TO M2 SITES IN OL AND CEN.

DISTRIBUTION OF MG AND FE OVER M1 AND M2 IN OL AND PYX FOLLOWS DAVIDSON AND LINDSLEY (ALSO DAVIDSON AND MUKHOPADHYAY, 1984, CMP, 86, P256). THE DISTRIBUTION OF MG AND FE OVER M1 AND M2 SITES IN OL AND CPX IS T AND P DEPENDENT AND BASED ON THE MINIMIZATION OF THE CHEMICAL POTENTIALS OF DI, HD, EN AND FS IN CPX OR EN.

REACTIONS:

1	 FORSTERITE+MELT=CLINOENSTATITE
2	 FAYALITE+MELT=FERROSILITE
3	 MONTICELLITE+MELT=DIOPSIDE

INPUT CONDITIONS:

INITIAL T(K) FINAL T(K) INCREMENTS INITIAL P(B) FINAL P(B) INCREMENTS

1173.2	1673.2	50.0	1.0	10001.0	1000.0
			LOGASI02		
P(B)	T(C)	(1)	(2)	(3)	
1.0	900.0	-0.38484	0.17757	-0.82288	
1.0	950.0	-0.34315	0.15484	-0.68064	
1.0	1000.0	-0.30837	0.13190	-0.54985	
1.0	1050.0	-0.27882	0.10899	-0.42923	
1.0	1100.0	-0.25332	0.08633	-0.31760	
1.0	1150.0	-0.23095	0.06400	-0.21406	
1.0	1200.0	-0.21103	0.04208	-0.11772	
1.0	1250.0	-0.19310	0.02063	-0.02791	
1.0	1300.0	-0.17673	-0.00037	0.05602	
1.0	1350.0	-0.16162	-0.02091	0.13464	
- 1.0	1400.0	-0.14754	-0.04101	0.20842	
1001 0	900 0	0 41525	0 15020	0 99005	
1001.0	950.0	-0.37158	0.13930		
1001.0	1000 0	-0.37138	0.13634	-0.61061	
- 1001 0	1050 0	-0.30368	0.11090	-0.48759	
1001 0	1100 0	-0.27664	0.07418	-0.37372	
1001.0	1150.0	-0.25284	0 05309	-0.26809	
1001.0	1200.0	-0.23161	0.03234	-0 16982	
1001.0	1250.0	-0.21246	0.01199	-0.07819	
1001.0	1300.0	-0.19494	-0.00798	0.00744	

-	1001.0 1001.0	1350.0 1400.0	-0.17877 -0.16368	-0.02755 -0.04671	0.08766 0.16295	
	2001.0 2001.0 2001.0 2001.0 2001.0 2001.0 2001.0 2001.0 2001.0 2001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.44390 -0.39818 -0.35977 -0.32695 -0.29845 -0.27334 -0.25088 -0.23060 -0.21202 -0.19484 -0.17883	$\begin{array}{c} 0.14301\\ 0.12354\\ 0.10360\\ 0.08347\\ 0.06339\\ 0.04346\\ 0.02379\\ 0.00445\\ -0.01457\\ -0.01457\\ -0.03323\\ -0.05153\end{array}$	-0.95301 -0.80529 -0.66943 -0.54413 -0.42815 -0.32056 -0.22045 -0.12709 -0.03984 0.04189 0.11861	
~	3001.0 3001.0 3001.0 3001.0 3001.0	900.0 950.0 1000.0 1050.0 1100.0	-0.47047 -0.42293 -0.38290 -0.34861 -0.31878	0.12846 0.11042 0.09181 0.07291 0.05396	-1.01477 -0.86451 -0.72633 -0.59888 -0.48089	
~	3001.0 3001.0 3001.0 3001.0 3001.0 3001.0	1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.29243 -0.26885 -0.24752 -0.22795 -0.20987 -0.19298	0.03508 0.01640 -0.00201 -0.02014 -0.03796 -0.05547	-0.37144 -0.26958 -0.17459 -0.08582 -0.00266 0.07542	
•	4001.0 4001.0 4001.0 4001.0 4001.0 4001.0 4001.0 4001.0 4001.0 4001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.49509 -0.44586 -0.36866 -0.33761 -0.31014 -0.28551 -0.26320 -0.24275 -0.22383 -0.20615	$\begin{array}{c} 0.11573\\ 0.09901\\ 0.08160\\ 0.06381\\ 0.04588\\ 0.02798\\ 0.01020\\ -0.00735\\ -0.02468\\ -0.04174\\ -0.05854 \end{array}$	-1.07433 -0.92169 -0.78131 -0.65181 -0.53195 -0.42073 -0.31724 -0.22071 -0.13050 -0.04598 0.03338	
~						
×.,	5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.51773 -0.46693 -0.42401 -0.38713 -0.35495 -0.32644 -0.30088 -0.27770 -0.25642 -0.23672 -0.21832	0.10485 0.08930 0.07297 0.05616 0.03919 0.02214 0.00519 -0.01160 -0.02821 -0.02821 -0.04458 -0.06071	-1.13166 -0.97679 -0.83436 -0.70295 -0.58131 -0.46844 -0.36341 -0.26544 -0.17387 -0.08808 -0.00752	
	6001.0 6001.0 6001.0 6001.0	900.0 950.0 1000.0 1050.0	-0.53840 -0.48619 -0.44201 -0.40398	0.09577 0.08128 0.06591 0.05001	-1.18680 -1.02982 -0.88547 -0.75228	

-	3001.0	1100.0	-0.65051	-1.98399
	3001.0	1150.0	-0.60224	-2.00551
	3001.0	1200.0	-0.55763	-2.02549
	3001.0	1250.0	-0.51631	-2.04415
	3001.0	1300.0	-0.47805	-2.06158
	3001.0	1350.0	-0.44248	-2.07791
	3001.0	1400.0	-0.40947	-2.09321
-	4001.0	900.0	-0.83551	-1.80778
	4001.0	950.0	-0.77037	-1.84005
	4001.0	1000.0	-0.71068	-1.86972
	4001.0	1050.0	-0.65583	-1.89715
	4001.0	1100.0	-0.60538	-1.92253
	4001.0	1150.0	-0.55887	-1.94609
	4001.0	1200.0	-0.51591	-1.96796
	4001.0	1250.0	-0.47615	-1.98837
	4001.0	1300.0	-0.43931	-2.00746
	4001.0	1350.0	-0.40514	-2.02533
	4001.0	1400.0	-0.37337	-2.04205
•	5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0 5001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.77981 -0.71720 -0.65986 -0.60721 -0.55877 -0.51416 -0.47293 -0.43479 -0.39948 -0.36674 -0.33633	-1.73482 -1.77001 -1.80235 -1.83223 -1.85989 -1.88558 -1.90941 -1.93168 -1.95247 -1.97194 -1.99018
-	6001.0 6001.0 6001.0 6001.0 6001.0 6001.0 6001.0 6001.0 6001.0 6001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.72215 -0.66224 -0.55701 -0.51069 -0.46806 -0.42868 -0.39225 -0.35857 -0.32730 -0.29830	-1.66024 -1.69843 -1.73358 -1.76602 -1.79606 -1.82395 -1.84982 -1.87400 -1.89660 -1.91775 -1.93755
•	7001.0 7001.0 7001.0 7001.0 7001.0 7001.0 7001.0 7001.0 7001.0 7001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.66255 -0.60546 -0.55320 -0.50525 -0.46118 -0.42058 -0.38317 -0.34852 -0.31650 -0.28685 -0.25934	-1.58405 -1.62536 -1.66338 -1.69853 -1.73103 -1.76120 -1.78922 -1.81538 -1.83983 -1.86275 -1.88420
-	8001.0	900.0	-0.60099	-1.50619
	8001.0	950.0	-0.54687	-1.55077
	8001.0	1000.0	-0.49736	-1.59181
	8001.0	1050.0	-0.45192	-1.62970

T (IN CELSIUS) = 900.00

-

^

_ _

FERRIC IRON AND FE3+ CALCULATED FROM CHARGE BALANCE

BERMAN THERMODYNAMIC DATA SET

NON-IDEAL PYROXENE, NON-IDEAL FELDSPAR

(1)	CATS + LIQ = AN
(2)	JAD + LIQ = ALE

			LOGASIO	2	
~	P(B)	Т(С)	(1)	(2)	
	1.0	900.0	-1.03899	-2.08323	
	1.0	950.0	-0.96493	-2.10514	
	1.0	1000.0	-0.89704	-2.12528	
	1.0	1050.0	-0.83464	-2.14391	
^	1.0	1100.0	-0.77718	-2.16115	
	1.0	1150.0	-0.72418	-2.17713	
	1.0	1200.0	-0.67515	-2.19196	
	1.0	1250.0	-0.62971	-2.20581	
	1.0	1300.0	-0.58762	-2.21876	
	1.0	1350.0	-0.54847	-2.23087	
-	1.0	1400.0	-0.51205	-2.24221	
	1001.0	900.0	-0.99105	-2.01680	
	1001.0	950.0	-0.91900	-2.04112	
	1001.0	1000.0	-0.85297	-2.06347	
	1001.0	1050.0	-0.79227	-2.08415	
-	1001.0	1100.0	-0.73640	-2.10327	
	1001.0	1150.0	-0.68490	-2.12103	
	1001.0	1200.0	-0.63724	-2.13749	
	1001.0	1250.0	-0.59310	-2.15286	
	1001.0	1300.0	-0.55220	-2.16725	
	1001 0	1350 0	-0 51417	-2 18068	
-	1001 0	1400 0	-0 47879	-2 19329	
	1001.0	1100.0	0.17072	2.19929	
	2001.0	900.0	-0.94113	-1.94873	
	2001.0	950.0	-0.87125	-1.97560	
	2001.0	1000.0	-0.80722	-2.00028	
	2001.0	1050.0	-0.74837	-2.02310	
-	2001.0	1100.0	-0.69419	-2.04421	
	2001.0	1150.0	-0.64425	-2.06382	
	2001.0	1200.0	-0.59807	-2.08200	
	2001.0	1250.0	-0.55529	-2.09896	
	2001.0	1300.0	-0.51567	-2.11486	
	2001.0	1350.0	-0.47885	-2.12970	
-	2001.0	1400.0	-0.44461	-2.14360	
	3001.0	900.0	-0.88932	-1.87909	
	3001.0	950.0	-0.82173	-1.90857	
	3001.0	1000.0	-0.75979	-1.93570	
	3001.0	1050.0	-0.70289	-1.96078	
-				=	

LOGASIO2							
P(B)	T(C)	(1)	(2)				
1.0	900.0	-1.04902	-2.05935				
1.0	950.0	-0.97494	-2.08163				
1.0	1000.0	-0.90702	-2.10212				
1.0	1050.0	-0.84459	-2.12106				
1.0	1150.0	-0.78710	-2.13860				
1.0	1200 0	-0.73408	-2.15480 -2 16994				
<u> </u>	1250.0	-0.63958	-2.18403				
1.0	1300.0	-0.59746	-2.19721				
1.0	1350.0	-0.55829	-2.20952				
1.0	1400.0	-0.52186	-2.22106				
1001.0	900.0	-1.00111	-1.99290				
1001.0	950.0	-0.92903	-2.01760				
1001.0	1000.0	-0.86297	-2.04030				
1001.0	1050.0	-0.80225	-2.06130				
1001.0	1150.0	-0.74634	-2.08071				
1001.0	1200.0	-0.69483	-2.09875				
-1001.0	1250.0	-0.60298	-2.11047				
1001.0	1300.0	-0.56206	-2.14568				
1001.0	1350.0	-0.52402	-2.15933				
1001.0	1400.0	-0.48862	-2.17213				
2001.0	900.0	-0.95122	-1.92484				
2001.0	950.0	-0.88130	-1.95208				
2001.0	1000.0	-0.81725	-1.97710				
2001.0	1050.0	-0.75837	-2.00024				
2001.0	1150 0	-0./0416	-2.02165				
2001.0	1200 0	-0.65419	-2.04153				
2001.0	1250 0	-0.56519	-2.05990				
2001.0	1300.0	-0.52556	-2.09329				
2001.0	1350.0	-0.48871	-2.10835				
2001.0	1400.0	-0.45445	-2.12244				
3001.0	900.0	-0.89944	-1.85519				
3001.0	950.0	-0.83181	-1.88504				
3001.0	1000.0	-0.76984	-1.91252				
3001.0	1050.0	-0.71291	-1.93791				
3001.0	1150.0	-0.66050	-1.96142				
3001.0	1200.0	-0.61220	-1.90322				
3001.0	1250.0	-0.52623	-2 02236				
3001.0	1300.0	-0.48795	-2.04001				
3001.0	1350.0	-0.45237	-2.05654				
3001.0	1400.0	-0.41933	-2.07204				
4001.0	900.0	-0.84565	-1.78387				
4001.0	950.0	-0.78048	-1.81651				
4001.0	1050.0	-0.72075	-1.84653				
4001.0 4001 0	1100 0	-0.66587	-1.8/428				
4001 0	1150 0	-0.01333	-1.07770				
4001.0	1200.0	-0.52588	-1.94591				

-	4001.0 4001.0 4001.0 4001.0	1250.0 1300.0 1350.0 1400.0	-0.48609 -0.44924 -0.41504 -0.38325	-1.96657 -1.98588 -2.00397 -2.02088	
-	5001.0 5001.0 5001.0 5001.0 5001.0	900.0 950.0 1000.0 1050.0 1100.0	-0.78997 -0.72733 -0.66996 -0.61727 -0.56881	-1.71090 -1.74647 -1.77916 -1.80935 -1.83732	
-	5001.0 5001.0 5001.0 5001.0 5001.0 5001.0	1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.52417 -0.48292 -0.44475 -0.40942 -0.37666 -0.34623	-1.86327 -1.88737 -1.90987 -1.93089 -1.95057 -1.96900	
-	6001.0 6001.0 6001.0 6001.0	900.0 950.0 1000.0 1050.0	-0.73234 -0.67239 -0.61750 -0.56710	-1.63631 -1.67488 -1.71038 -1.74314	
~	6001.0 6001.0 6001.0 6001.0 6001.0 6001.0	1100.0 1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.52075 -0.47809 -0.43868 -0.40223 -0.36853 -0.33724 -0.30822	-1.77347 -1.80164 -1.82777 -1.85218 -1.87501 -1.89637 -1.91638	
-	7001.0 7001.0 7001.0 7001.0 7001.0	900.0 950.0 1000.0 1050.0 1100.0	-0.67276 -0.61564 -0.56335 -0.51536 -0.47126	-1.56012 -1.60181 -1.64018 -1.67565 -1.70844	
-	7001.0 7001.0 7001.0 7001.0 7001.0	1200.0 1250.0 1300.0 1350.0 1400.0	-0.39319 -0.35852 -0.32648 -0.29680 -0.26927	-1.73889 -1.76717 -1.79357 -1.81824 -1.84137 -1.86301	
1	8001.0 8001.0 8001.0 8001.0 8001.0	900.0 950.0 1000.0 1050.0 1100.0	-0.61123 -0.55707 -0.50753 -0.46205 -0.42027	-1.48226 -1.52721 -1.56859 -1.60681 -1.64220	
-	8001.0 8001.0 8001.0 8001.0 8001.0 8001.0	1150.0 1200.0 1250.0 1300.0 1350.0 1400.0	-0.38184 -0.34639 -0.31365 -0.28337 -0.25532 -0.22934	-1.67503 -1.70553 -1.73401 -1.76063 -1.78554 -1.80889	
	9001.0 9001.0 9001.0 9001.0 9001.0 9001.0 9001.0	900.0 950.0 1000.0 1050.0 1100.0 1150.0 1200.0	-0.54774 -0.49669 -0.44999 -0.40716 -0.36783 -0.33166 -0.29835	-1.40275 -1.45110 -1.49560 -1.53671 -1.57473 -1.61004 -1.64287	

ENTHALPY AND ENTROPY OF FUSION CALCULATED FROM DATA OF RICHET ET AL. (GCA, 1982) AND DATA OF BERMAN FOR B-QTZ. VOLUMES OF SILICA MELT CALCULATED USING DATA OF KRESS AND CARMICHAEL (CMP, 1991). ACTIVITIES OF AN AND AB CALCULATED USING METHOD OF FUHRMAN AND LINDSLEY (AM MIN, 1989). ACTIVITIES OF CATS AND JD CALCULATED USING METHOD OF ANOVITZ (AM MIN, 1991) AND AN IDEAL SOLUTION MODEL IS ALSO USED.									
INITIAL	CONDITI	ONS							
INITIAL 1.0	P F 1	'INAL P .0001.0	INCRI 1000	EMENTS (1	P IN BARS	5)			
T (IN CE	LSIUS)	= -273.	15						
BERMAN T	HERMODY	NAMIC DA	TA SET						
NON-IDEA	L PYROX	ENE, NON	-IDEAL H	FELDSPAR					
(1) (2)			CATS JAD	5 + LIQ = + LIQ =	= AN ALB				
-	- (-)		LOC	GASIO2	. ,				
Р(В) 	·T (C)		(1)	(2	2) 				
DATA FOR	SAMPLE	TODD 5							
PYROX	ENE	WITH	CALCULA	ATED FE3-	+	PLA	GIOCLASE		
SIO2 AL2O3 TIO2 CR2O3 FE2O3 FEO MNO MGO CAO NA2O SUM	48.86 10.36 0.50 0.02 0.00 8.49 0.29 11.92 18.14 1.41 99.99	SI AL TI CR FE3+ FE2+ MN MG CA NA SUM MGNO -	1.802 0.450 0.014 0.001 0.262 0.009 0.655 0.716 0.101 4.010 0.714	SI AL TI CR FE3+ FE2+ MN MG CA NA SUM MGNO -	0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	SIO2 AL2O3 FEO MGO CAO NA2O K2O BAO SUM	43.44 35.30 0.63 0.00 18.91 0.74 0.02 0.00 99.04	SI AL FE MG CA NA K BA SUM	2.035 1.949 0.025 0.000 0.948 0.067 0.001 0.000 5.025
		EN = FS = WO =	0.401 0.160 0.439	EN = FS = WO =	= 0.000 = 0.000 = 0.000			AN = (AB = (OR = (CS =	0.933 0.066 0.001 0

PYROXENE MOLE FRACTIONS KNAM2 = .1005651

References

Barton M, Wyers, G.P (1991) Estimates of P, T, P_{H2O} and f_{O2} for lavas from Patmos (Greece) and implications for magmatic evolution. Jour. of Volcanology and Geothermal Res., 47: 265-297

Barton M. Estimating the conditions of crystallization of magmas. unpublished: 1-14

- Berman RG. (1991) Thermobarometry using multi-equilibrium calculations: A new technique with petrological applications. Canadian Mineralogist 29: 833-855
- Huijsmans, J.J.P. and Barton, M., (1989) Geochemical evolution of two shield volcanoes from Santorini, Aegean Sea, Greece: Evidence for zoned magma chambers from cyclic compositional variations. Jour. of Petrology 30: 583-625
- Lange, R.L. and Carmichael, I.S.E., (1990) Thermodynamic properties of silicate liquids with emphasis on density, thermal expansion and compressibility. Reviews in Mineralogy 24:25-64.
- MacCracken, L. (1993) An estimate of P,T, and water content for a lava from Santorini and thermodynamic applications. Senior Thesis: 1-14