

In the application of equilibrium thermodynamics, we take the starting point to be what I call the “equilibrium relationship”: the relationship for a balanced chemical reaction between the end-members of phases that are in equilibrium with each other:

$$0 = \Delta G^o + RT \ln K \quad (1)$$

in which  $\Delta G^o$  is the Gibbs energy of the reaction between the pure end-members in the same structure as the phases in which they occur,  $K$  is the equilibrium constant, in terms of the activities of the end-members in their phases,  $T$  is temperature, and  $R$  is the gas constant.

Looking at (1), the first practical concern is where we get the numbers from to insert into  $\Delta G^o$  for any particular reaction. There are actually two sides to this: the form that the Gibbs energies of pure end-members should have as a function of  $P$  and  $T$ , and what the numbers are. These two go hand-in-hand, and in the context of the internally-consistent dataset that THERMOCALC uses, the papers to read are

Powell, R, and Holland, TJB, 1985 An internally consistent thermodynamic dataset with uncertainties and correlations : 1 : Methods and a worked example. *Journal of Metamorphic Geology* **3**, 327–342.

Holland, TJB, and Powell, R, 1985 An internally consistent thermodynamic dataset with uncertainties and correlations : 2 : Data and results. *Journal of Metamorphic Geology* **3**, 343–370.

Holland, TJB, and Powell, R, 1990 An enlarged and updated internally consistent thermodynamic dataset with uncertainties and correlations: the system  $K_2O$ - $Na_2O$ - $CaO$ - $MgO$ - $MnO$ - $FeO$ - $Fe_2O_3$ - $Al_2O_3$ - $TiO_2$ - $SiO_2$ - $C$ - $H_2$ - $O_2$ . *Journal of Metamorphic Geology* **8**, 89–124.

Powell, R, and Holland, TJB, 1993. Is Least Squares an appropriate methodology to be used in the extraction of thermodynamic data from experimentally-bracketed mineral equilibria? *American Mineralogist*, **78**, 107–112.

Holland, TJB, and Powell, R, 1998. An internally-consistent thermodynamic dataset for phases of petrological interest. *Journal of Metamorphic Geology* **16**, 309–344.

How much of this you should read depends very much on how much you really think you need to know. If you are going to use THERMOCALC datafiles that we provide, there may be little point getting too involved. If, however, you want to fiddle with the data (via DQF) it is as well to have a clear understanding of the correlations within the data, and also what is *assumed* about activity-composition relationships in the data (as spelt out most clearly in the 1998 paper). If you are interested just in our philosophy of data extraction from experimental work, start with the 1993 paper. If you want to know more, having read the 1993 paper, continue with the 1998 paper, going to the earlier papers if there is something that you don’t understand otherwise.

## A brief outline

Whereas there is no substitute for reading the papers, two paragraphs extracted from the papers bring out some of what we have developed and what we follow. From the introduction of the Holland and Powell (1998) paper:

The thermodynamic data extraction involves using weighted least squares on the different types of data (calorimetric, phase equilibria, natural mineral partitioning) to determine enthalpies of formation of the end-members of the phases. Entropies, volumes, heat capacities, thermal expansions and compressibilities are not derived by regression, but are taken as known in this process. Other parameters intimately involved, for example regular solution parameters in exchange equilibria, are also taken as known, having been determined separately by pre-processing the data. The entropies of the end-members in the data set are not determined along with the enthalpies by regression because, in most circumstances, they are determined more reliably by estimation techniques (e.g. Holland, 1989) than by fitting to experimental brackets. Where appropriate, such estimated entropies have been adjusted, within their likely uncertainties, to improve agreement with the experiments. The regression involves determination of the enthalpies of 189 end-members using 319 reaction equilibria, 82 direct calorimetric constraints on the end-member enthalpies of formation at 298 K, and 30 constraints from enthalpies of reaction and high-temperature calorimetry. Thus the total number of degrees of freedom in the regression is  $242 (319 + 82 + 30 - 189)$ , and the value for  $\sigma_{\text{fit}}$  is 1.14.

The abstract of the Powell & Holland (1993) encapsulates the least squares philosophy that has been followed in dataset generation, written in the context of some criticisms in the literature of our approach to constraining thermodynamic data using experimental data:

The applicability of least squares in the extraction of thermodynamic data from experimentally-bracketed mineral equilibria is considered primarily as a statistical (and logical) problem concerning the nature of the experimental data, and the nature of the information which is to be extracted. The former relates particularly to the bracketed nature of the data, the latter to the requirement that not only thermodynamic data, but also the uncertainties on, and the correlations between the data, are to be extracted. By examining the probability distributions, it is shown that the majority of experimental brackets are approximately Gaussian distributed, primarily because experimental brackets are not generally very wide compared with experimental uncertainties on the bracket ends. Thus, using least squares on all the experimental brackets would be apposite for the thermodynamic data extraction problem. However, rather than fitting all the experimental brackets, we fit composite data formed from the individual experimental brackets for each experimentally-determined reaction. It is shown that the use of composite data is equivalent to using all the brackets as long as the composite data are determined appropriately. The main reason for wishing to use composite data is that it allows the deleterious effect on the least squares caused by inconsistent brackets to be minimised. The uncertainties on very few of the composite data are large compared with

the uncertainties on the ends of individual brackets. Therefore, least squares on composite data is appropriate for data extraction. Moreover much of the uncertainty on the extracted thermodynamic data comes from uncertainty on the position of the bracket ends rather than the width of the brackets themselves.

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The following table shows the results of the least squares fitting by the program LSQDS on the body of experimental data used to generate the 1998 dataset (Holland & Powell, 1998, Table 7). Tim Holland regularly (continuously) upgrades the dataset, and the version we use in the Workshop is one from Sept 19, 1999, which is a minor upgrade of the Holland & Powell (1998), except that the new silicate model data is included (Holland & Powell, 2001), and the amphibole data are consistent with Dale et al. (2000). RP wrote and maintains the LSQDS software.

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Holland and Powell (1998) An internally consistent thermodynamic dataset for phases of petrological interest. *Journal of Metamorphic Geology*.

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TABLE 7b: The experimental data used in setting up the least squares problem for solving for the enthalpies of formation of the phases in LSQDS, and the results of the least squares analysis. The experimental data are grouped according to chemical subsystems: (click on system below to go to relevant page for details)

<a href="#">SiO<sub>2</sub> + CaO–SiO<sub>2</sub></a>	<a href="#">MgO–SiO<sub>2</sub></a>
<a href="#">CaO–MgO–SiO<sub>2</sub></a>	<a href="#">Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">CaO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	<a href="#">MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	<a href="#">Na<sub>2</sub>O–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">K<sub>2</sub>O–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	<a href="#">K<sub>2</sub>O–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">Na<sub>2</sub>O–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub> + K<sub>2</sub>O–CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	
<a href="#">Na<sub>2</sub>O–CaO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub> + Na<sub>2</sub>O–CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	
<a href="#">FeO–SiO<sub>2</sub></a>	<a href="#">FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">Na<sub>2</sub>O–FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub> + K<sub>2</sub>O–FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>	<a href="#">CaO–FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub></a>
<a href="#">Osumilite + KFMASH melt equilibria</a>	<a href="#">Ni–Ti–Zr–bearing equilibria</a>
<a href="#">Exchange equilibria</a>	<a href="#">Mn–equilibria</a>
<a href="#">Melting equilibria</a>	

The first columns give the experimental data, in the form of the P, T, x(CO<sub>2</sub>) and ln K of the experiments, followed by the corresponding enthalpies of reaction calculated using the entropies, volumes etc in Table 5. LSQDS converts the enthalpies of reaction into an enthalpy of reaction bracket given in the first line of the summary. The least squares enthalpy of reaction (cH) is given in the second line of the summary, with its calculated uncertainty. The calc column gives the calculated T, P or ln K of the experimental conditions using the least squares results, followed by its uncertainty. The miss column gives the amount that the calculated T, P or ln K is outside the experimental bracket (if at all). In the summary information for each reaction, the code on the first line relates to the calculation of the enthalpy of reaction bracket (see Powell and Holland, 1993); the number at the end of the second line (if present) is a factor used in weighting experimental results in the least squares analysis; the comment making up the third line gives an overall appraisal of the relationship between the enthalpy of reaction bracket and the calculated enthalpy of reaction; uH on the fourth line is a measure of the uncertainty on each end of the enthalpy of reaction bracket arising from experimental uncertainties (in P, T etc), d/s is a measure of bracket overlap normalised to the uncertainty on bracket ends as discussed in Powell and Holland (1993), and h is the hat matrix diagonal.

## SiO<sub>2</sub> & CaO-SiO<sub>2</sub>

1) **diam = gph** (Kennedy & Kennedy, 1976)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	47.0 46.0	1100	-2.10	-1.95	miss	46.83	0.98	3 (-2.24 <-> -1.90)
0	-	50.0 49.0	1200	-2.13	-1.98		49.61	1.00	cH = -2.07 (sd 0.07)
0	-	53.0 52.0	1300	-2.17	-2.03		52.31	1.01	within bracket
0	-	56.0 54.0	1400	-2.23	-1.95		54.88	1.02	uH = 0.14, d/s = 0.2, h = 1.00
0	-	58.0 57.0	1500	-2.17	-2.03		57.32	1.03	
0	-	60.0 59.0	1600	-2.13	-1.99		59.60	1.05	

2) **q = trd** (Ostrovsky, 1966)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	864 870	4.14	4.15	miss	867	12	2 (4.14 <-> 4.16)
0	-	1.0	1040 1090	4.10	4.18		1070	12	cH = 4.15 (sd 0.01)
									within bracket
									uH = 0.01, d/s = 0.6, h = 0.98

3) **trd = crst** (Ostrovsky, 1966)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1465 1475	0.70	0.70	miss	1468	12	2 (0.69 <-> 0.70)
0	-	1.0	1220 1260	0.68	0.70		1257	12	cH = 0.70 (sd 0.00)
									within bracket
									uH = 0.00, d/s = 0.5, h = 1.00

4) **q = crst** (Ostrovsky, 1966; Jackson, 1976)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	2.2 1.6	1300	4.90	5.05	0.24	2.44	0.06	2 (4.85 <-> 4.91)
0	-	7.0	1730	4.43			2040	16	cH = 4.84 (sd 0.01)
0	-	5.0	1690		4.85		1684	14	too low but OK
									uH = 0.02, d/s = -1.3, h = 0.02

5) **coe = q** (Bose & Ganguly, 1995)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	27.6 26.9	500	-5.37	-5.24	miss	27.55	0.58	3 (-5.51 <-> -5.24)
0	-	28.4 27.6	600	-5.46	-5.30		27.93	0.58	cH = -5.37 (sd 0.05)
0	-	29.0 28.3	700	-5.48	-5.34		28.41	0.59	within bracket
0	-	29.8 29.0	800	-5.53	-5.37	-0.00	29.00	0.60	uH = 0.11, d/s = 0.0, h = 0.95
0	-	30.3 29.6	900	-5.49	-5.34		29.70	0.61	
0	-	31.1 29.9	1000	-5.48	-5.24		30.52	0.62	
0	-	31.7 30.9	1100	-5.41	-5.25		31.46	0.63	
0	-	32.6 31.8	1200	-5.38	-5.21		32.53	0.64	

\* **coe = q** (Bohlen & Boettcher, 1982; Gasparik, 1984)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	24.9 24.5	400	-4.90	-4.82	2.37	27.27	0.57	** NOT USED **
0	-	25.7 25.3	500	-5.00	-4.92	1.85	27.55	0.58	cH = -5.37 (sd 0.05)
0	-	26.6 26.1	600	-5.10	-5.00	1.33	27.93	0.58	
0	-	27.3 26.7	700	-5.14	-5.02	1.11	28.41	0.59	
0	-	28.1 27.7	800	-5.18	-5.10	0.90	29.00	0.60	
0	-	28.8 28.4	900	-5.18	-5.10	0.90	29.70	0.61	
0	-	29.9 29.4	1000	-5.24	-5.13	0.62	30.52	0.62	
0	-	31.1 30.6	1100	-5.29	-5.18	0.36	31.46	0.63	

6) **stv = coe** (Zheng et al., 1996)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	90.6 87.0	1100	-31.14	-29.22	miss	88.15	2.13	3 (-30.99 <-> -28.67)
0	-	93.2 90.4	1200	-30.76	-29.28		91.45	2.15	cH = -29.84 (sd 0.57)
0	-	96.3 93.0	1300	-30.61	-28.89		94.82	2.17	within bracket
0	-	97.6	1430		-28.97		1381	64	uH = 0.98, d/s = 0.7, h = 0.61
0	-	100.4	1530		-28.61		1462	64	

7) arag = cc (Johannes & Puhan, 1971; Crawford & Hoersch, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	4.1	70 90	-0.08	-0.00	31	121	14	5 (0.04 <-> 0.19)
0	-	5.0	160 200	0.04	0.21		178	12	cH = 0.11 (sd 0.03)
0	-	7.0	280 320	0.07	0.26		289	12	within bracket
0	-	9.0	380 420	0.08	0.28		387	12	uH = 0.04, d/s = -1.0, h = 0.95
0	-	11.0	460 500	0.03	0.23		477	10	
0	-	13.0	540 580	-0.00	0.20		562	10	
0	-	15.0	600 640	-0.11	0.10	3	643	10	

8) arag = cc (Irving & Wyllie, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	20.0 19.0	800	-0.02	0.16		19.25	0.31	3 (-0.04 <-> 0.16)
0	-	25.6 24.7	950	-0.15	-0.01	-0.80	23.90	0.35	cH = 0.11 (sd 0.03) 2
0	-	30.5 29.5	1100	-0.00	0.13		29.64	0.41	within bracket
									uH = 0.09, d/s = -0.1, h = 0.05

9) wo = psw (Osborne & Shairer, 1941; Huang & Wyllie, 1975)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1115 1135	6.34	6.41		1124	16	1 (6.34 <-> 6.40)
0	-	22.0 21.0	1550	6.32	6.40		21.37	0.69	cH = 6.37 (sd 0.03)
									within bracket
									uH = 0.03, d/s = 1.1, h = 0.99

10) cc = lime + CO2 (Smyth & Adams, 1923; Baker, 1962)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	0.0	930 950	176.81	179.51		947	6	3 (178.92 <-> 180.81)
0	1	0.0	1035 1065	178.91	182.62		1036	6	cH = 179.09 (sd 0.37)
0	1	0.0	1065 1095	179.42	183.05	-3	1062	6	within bracket
0	1	0.0	1140 1160	178.30	180.57		1147	6	uH = 0.68, d/s = 0.1, h = 0.54
0	1	0.0	1210 1230	178.66	180.81		1214	6	
0	1	0.0	1230 1250	179.13	181.26		1230	6	

11) cc + q = wo + CO2 (Zhu, Newton & Kleppa, 1993)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	2.3 1.9	700	88.66	90.51	-0.07	1.83	0.08	3 (89.49 <-> 90.50)
0	1	3.1 2.7	750	89.25	90.77	-0.02	2.68	0.10	cH = 90.86 (sd 0.20)
0	1	4.1 3.8	800	89.45	90.41	-0.14	3.66	0.12	too high but OK
0	1	5.2 4.9	850	89.63	90.46	-0.14	4.76	0.13	uH = 0.43, d/s = 0.9, h = 0.36

12) cc + q = wo + CO2 (Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.86	6.0	870 890	90.30	91.61		879	6	1 (90.34 <-> 91.56)
0	1	6.0	890 915	90.18	91.77		901	6	cH = 90.86 (sd 0.20)
									within bracket
									uH = 0.44, d/s = 1.5, h = 0.15

\* cc + q = wo + CO2 (Ziegenbein & Johannes, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	2.0	690 710	89.24	90.80	1	711	6	** NOT USED **
0	1	4.0	790 810	89.07	90.46	6	816	6	cH = 90.86 (sd 0.20)
0	1	6.0	895 915	90.50	91.77		901	6	

\*  $cc + q = wo + CO_2$  (Greenwood, 1967; Harker & Tuttle, 1955)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	1.0	662	685	93.05	95.02	-26	636	4	** NOT USED **
0	0.69	1.0	640		93.82		-33	607	4	cH = 90.86 (sd 0.20)
0	0.72	1.0		660		95.31		610	4	
0	1	2.0	725	750	91.97	93.91	-14	711	6	
0	0.80	2.0	700	711	91.77	92.65	-11	689	6	
0	0.50	2.0	658	679	91.38	93.16	-6	652	4	
0	1	1.0	650	690	92.03	95.45	-14	636	4	
0	1	2.0	730	750	92.36	93.91	-19	711	6	
0	1	2.7	780	800	92.99	94.46	-29	751	6	

13)  $cc + q = wo + CO_2$  (Haselton et al., 1978)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	9.3	1000	1015	89.84	90.68	3	1018	8	3 (89.84 <-> 90.99)
0	1	15.0	1175	1200	89.92	91.16		1194	8	cH = 90.86 (sd 0.20) 2
0	1	19.0	1300	1325	90.59	91.75		1306	8	within bracket
0	1	10.2 9.3	1015		89.05	90.68	-0.10	9.20	0.20	uH = 0.49, d/s = 0.1, h = 0.08

14)  $3cc + 2wo = ty + CO_2$  (Zharikov & Shmulovich, 1969)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	0.1	800	830	125.67	128.82		830	6	3 (127.91 <-> 129.11)
0	1	0.2	880	890	127.27	128.23	7	897	6	cH = 128.86 (sd 0.31)
0	1	0.3	950	960	128.34	129.21		956	8	within bracket
0	1	0.4	960	980	128.02	129.69		970	8	uH = 0.51, d/s = -0.1, h = 0.90
0	1	0.5	990	1000	128.17	128.98		998	8	

15)  $ty = spu + CO_2$  (Zharikov & Shmulovich, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	0.1	850	860	123.40	124.40	7	867	6	3 (124.17 <-> 125.36)
0	1	0.2	930	940	124.32	125.24		939	6	cH = 125.13 (sd 0.32)
0	1	0.2	950	980	124.28	126.98		959	6	within bracket
0	1	0.3	990	1000	124.14	125.00	1	1001	8	uH = 0.51, d/s = -0.4, h = 0.89
0	1	0.5	1040	1060	124.79	126.44		1044	8	

16)  $spu + 4wo = 3rnk + CO_2$  (Zharikov & Shmulovich, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	0.1	850	870	156.80	159.34		867	14	2 (158.07 <-> 159.89)
0	1	0.2	920	940	158.62	161.00		923	14	cH = 158.98 (sd 0.84)
										within bracket
										uH = 0.65, d/s = 0.6, h = 1.00

17)  $spu + rnk = 4lrn + CO_2$  (Zharikov & Shmulovich, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	0.1	900	910	170.46	171.93		908	10	3 (170.77 <-> 172.50)
0	1	0.1	935	960	170.51	174.10		943	10	cH = 171.64 (sd 0.67)
0	1	0.2	980	1000	169.83	172.60		993	10	within bracket
0	1	0.3	1020	1050	171.08	175.17		1024	10	uH = 0.74, d/s = 0.6, h = 1.00

## MgO-SiO<sub>2</sub>

18) **ta + 2en = anth** (Chernosky et al., 1985)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	10.0	755 780	8.39	8.79	3	783	18	1 (8.41 <-> 8.77) cH = 8.85 (sd 0.15) too high but OK uH = 0.13, d/s = 1.6, h = 0.51

19) **phA = 3br + 2fo** (Pawley & Wood, 1995)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	27.5 26.0	500	10.88	11.54		26.67	2.27	3 (10.88 <-> 11.61)
0	-	34.8 32.5	600	11.04	11.95		34.29	2.63	cH = 11.24 (sd 0.51) 2
0	-	39.5 37.5	650	10.88	11.58		38.46	2.87	within bracket uH = 0.30, d/s = 0.8, h = 1.00

20) **br = per + H<sub>2</sub>O** (Barnes & Ernst, 1963;)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	564 574	80.87	81.60		573	4	3 (81.10 <-> 81.80)
0	0	1.0	604 607	80.99	81.18	5	612	4	cH = 81.51 (sd 0.14) 2
0	0	1.5	633 648	81.31	82.16		637	6	within bracket
0	0	2.0	653 664	81.35	81.94		656	6	uH = 0.30, d/s = -0.3, h = 0.13

21) **br = per + H<sub>2</sub>O** (Aranovich & Newton, 1995)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	655 670	81.46	82.26		656	6	3 (81.23 <-> 81.86)
0	0	4.2	715 730	81.23	81.93		721	6	cH = 81.51 (sd 0.14)
0	0	7.0	770 790	80.98	81.82		783	8	within bracket
0	0	10.0	830 845	81.29	81.87		836	8	uH = 0.25, d/s = 0.0, h = 0.77
0	0	15.0	890 905	80.93	81.46	1	906	8	

22) **br = per + H<sub>2</sub>O** (Schramke et al., 1981; Irving et al., 1977)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	690 725	80.29	81.93		716	6	1 (80.81 <-> 81.50)
0	0	5.1	720 745	80.50	81.62		743	6	cH = 81.51 (sd 0.14) 2
0	0	6.1	740 765	80.46	81.54		764	6	too high but OK
0	0	8.1	785 806	80.77	81.62		803	8	uH = 0.24, d/s = 1.6, h = 0.08

\* **br = per + H<sub>2</sub>O** (Irving et al., 1977)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	17.0	915 945	80.99	82.02		930	8	** NOT USED **
0	0	27.0	1020 1080	81.45	83.31		1022	10	cH = 81.51 (sd 0.14)
0	0	33.0	1075 1105	81.93	82.83	-14	1061	10	

23) **2ta = 3en + 2q + 2H<sub>2</sub>O** (Chernosky, 1976; Chernosky et al., 1985; Skippen, 1971)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	656 672	216.19	219.55		663	2	3 (217.26 <-> 219.44)
0	0	1.0	700 721	218.16	222.18	-3	697	2	cH = 217.66 (sd 0.27)
0	0	2.0	725 735	217.03	218.77		729	4	within bracket uH = 0.93, d/s = 0.3, h = 0.10

24) **2ta = 3en + 2q + 2H<sub>2</sub>O** (Chernosky et al., 1985)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	10.0	790 800	215.93	217.35	2	802	4	3 (214.48 <-> 216.14)
0	0	13.0	800		216.01	12	812	4	cH = 217.66 (sd 0.27)
0	0	13.6	785	213.80			814	4	too high
0	0	17.0	795	214.39			820	4	uH = 0.70, d/s = 0.1, h = 0.08



25) 2ta = 3en + 2q + 2H2O (Jenkins, Holland & Clare, 1991)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	25.0	800	820	214.34	216.78	7	827	4	1 (214.54 <-> 216.57)
0	0	28.0	770		210.69			829	4	cH = 217.66 (sd 0.27)
										too high
										uH = 0.61, d/s = 2.0, h = 0.05

\* 2ta = 3en + 2coe + 2H2O (Pawley & Wood, 1995)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	29.0	800	820	224.96	227.28	10	830	6	** NOT USED **
0	0	38.0	770	790	224.99	227.18	11	801	6	cH = 228.40 (sd 0.29)
0	0	49.0		730		224.48	38	768	6	

26) 2fo + 2ta = 5en + 2H2O (Chernosky, 1976; Chernosky et al., 1985)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	600	621	198.70	202.93		619	2	3 (201.46 <-> 203.75)
0	0	1.0	652	657	203.38	204.29	-4	648	4	cH = 202.61 (sd 0.30)
0	0	2.0	650	677	199.44	203.85		669	4	within bracket
0	0	3.0	673	692	201.56	204.53		680	4	uH = 0.97, d/s = -0.2, h = 0.36
0	0	4.0	686	691	202.72	203.48	-1	685	4	
0	0	6.0	679	694	201.21	203.36		689	4	

27) 2anth = 7en + 2q + 2H2O (Chernosky & Autio, 1979)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	719	760	197.50	204.02		735	6	3 (199.00 <-> 200.74)
0	0	1.5	752	767	199.28	201.51		757	6	cH = 199.97 (sd 0.40)
0	0	2.0	765	775	199.10	200.51		771	6	within bracket
0	0	3.0	755		195.37			790	6	uH = 0.74, d/s = 0.8, h = 0.30
0	0	10.0		815		200.77		808	8	

28) 7ta = 3anth + 4q + 4H2O (Chernosky & Autio, 1979)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	647	677	462.24	476.28	-1	646	2	3 (461.85 <-> 466.56)
0	0	1.0	664	687	456.41	466.24		677	4	cH = 461.87 (sd 0.70)
0	0	1.5	693	701	461.61	464.86		694	4	within bracket
0	0	2.0	706	719	461.90	467.02		706	4	uH = 2.00, d/s = 0.5, h = 0.22
0	0	3.0	727	742	462.72	468.39	-2	725	4	

29) 2anth + 2fo = 9en + 2H2O (Chernosky et al., 1985)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	632	667	183.21	189.20		642	6	1 (183.29 <-> 185.32)
0	0	2.0	677	710	181.86	186.26		700	6	cH = 184.92 (sd 0.43)
0	0	4.0	677		181.26			708	8	within bracket
0	0	5.0	684	735	182.64	188.54		704	8	uH = 0.72, d/s = 1.5, h = 0.14
0	0	6.0	661	701	180.93	185.40		697	8	

30) 9ta + 4fo = 5anth + 4H2O (Chernosky et al., 1985)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	625	645	450.19	458.97	-2	623	4	3 (447.63 <-> 453.25)
0	0	2.0	635	660	445.66	455.75		644	4	cH = 449.45 (sd 0.93)
0	0	5.0	665	685	445.49	452.89		676	6	within bracket
0	0	6.0	674	689	446.30	451.76		683	6	uH = 2.02, d/s = 0.4, h = 0.27

31)  $br + chr = 2fo + 3H_2O$  (Johannes, 1968; Kitahara et al., 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	350 370	212.99	216.17		358	4	1 (213.71 <-> 215.64)
0	0	3.0	380 400	213.26	215.80		388	6	cH = 214.29 (sd 0.52)
0	0	4.0	395 430	213.55	218.80		401	4	within bracket
0	0	7.0	415 440	212.60	216.31		427	8	uH = 0.61, d/s = 1.8, h = 0.48
0	0	18.2	450 520	210.33	219.40		481	8	
0	0	27.3	460 520	209.12	216.39		503	10	

32)  $5chr = ta + 6fo + 9H_2O$  (Chernosky, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	456 476	680.54	690.52		471	10	1 (682.38 <-> 689.97)
0	0	5.0	468 488	681.83	691.53		481	10	cH = 687.95 (sd 2.53)
									within bracket
									uH = 2.50, d/s = 1.7, h = 0.58

33)  $atg = 4ta + 18fo + 27H_2O$  (Evans et al., 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	480 540	2122.22	2222.55		531	8	3 (2198.23 <-> 2217.92)
0	0	4.0	520 570	2144.07	2220.72		562	10	cH = 2208.07 (sd 7.18)
0	0	6.0	560 590	2173.44	2216.89		584	10	within bracket
0	0	10.0	615 630	2207.15	2227.17		616	10	uH = 7.17, d/s = 0.7, h = 1.00
0	0	15.0	640 660	2205.88	2230.75		642	12	

34)  $2cumm = 7en + 2q + 2H_2O$  (Fonarev & Korolkov, 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.79	0	3.0	718 748	174.75	178.25		732	24	2 (174.66 <-> 178.07)
0.64	0	5.0	728 758	174.73	177.99		743	26	cH = 176.37 (sd 1.39)
									within bracket
									uH = 1.35, d/s = 1.2, h = 1.00

35)  $chum = 4fo + per + H_2O$  (Duffy & Greenwood, 1979)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.43	0	2.0	751	106.31	107.62		0.43	0.16	1 (106.37 <-> 107.56)
									cH = 106.97 (sd 0.68)
									within bracket
									uH = 0.41, d/s = 1.6, h = 1.00

36)  $mag = per + CO_2$  (Harker & Tuttle, 1955; Goldsmith & Heard, 1962)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	0.7	730 750	116.38	118.48		731	4	3 (116.53 <-> 117.99)
0	1	1.4	800 825	116.74	119.17	-3	797	4	cH = 116.43 (sd 0.23)
0	1	2.1	800 875	112.30	119.23		845	6	too low but OK
0	1	2.8	875 900	115.59	117.81		885	6	uH = 0.52, d/s = 1.0, h = 0.19
0	1	3.0	952		121.43		895	6	
0	1	5.0	977 1008	115.61	118.14		987	6	

37)  $mag = per + CO_2$  (Johannes & Metz, 1968; Philipp & Girsperger, 1990; Koziol & Newton, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	0.5	680 710	113.91	117.18		703	4	3 (115.43 <-> 116.68)
0	1	1.0	740 760	114.14	116.16	3	763	4	cH = 116.43 (sd 0.23)
0	1	2.0	810 835	113.79	116.12	3	838	6	within bracket
0	1	0.5	700 710	116.09	117.18		703	4	uH = 0.53, d/s = -0.0, h = 0.44
0	1	0.6 0.6	715	115.86	116.75		0.58	0.03	
0	1	1.0	760 770	116.16	117.17		763	4	

\* mag = per + CO2 (Irving & Wyllie, 1975)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	18.0	1350 1400	114.25	117.46		1384	8	** NOT USED **
0	1	21.0	1420 1470	114.00	117.09		1459	8	cH = 116.43 (sd 0.23)
0	1	22.7	1520		117.59		1501	8	

\* 2mag + 2q = en + 2CO2 (Johannes, 1969)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	2.0	510 520	168.19	170.08	-3	507	4	** NOT USED **
									cH = 167.66 (sd 0.40)

38) 2mag + 2q = en + 2CO2 (Koziol & Newton, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	7.5	638 663	162.73	166.75	6	669	4	5 (166.59 <-> 170.42)
0	1	8.0	640 670	161.30	166.09	10	680	4	cH = 167.66 (sd 0.40)
0	1	10.6 10.2	715	164.81	166.00	-0.54	9.66	0.24	within bracket
0	1	12.0	750 782	166.11	170.90		760	6	uH = 1.02, d/s = -1.9, h = 0.38
0	1	14.0	801 820	168.35	171.12	-5	796	6	
0	1	15.5	816 851	166.81	171.82		822	6	
0	1	17.5	870 890	169.82	172.61	-15	855	6	

\* 2mag + 2coe = en + 2CO2 (Haselton et al., 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	37.0	1120 1140	154.54	157.02		1139	6	** NOT USED **
0	1	41.6	1185 1200	154.21	156.02	8	1208	6	cH = 156.93 (sd 0.41)

39) 2mag + en = 2fo + 2CO2 (Haselton et al., 1978; Koziol, 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	8.0	740 780	177.06	183.45		775	6	3 (179.96 <-> 183.74)
0	1	10.0	810 830	179.53	182.60	1	831	6	cH = 182.72 (sd 0.41)
0	1	14.0	930 950	182.22	185.09		933	6	within bracket
0	1	17.6	1000 1020	179.94	182.67		1020	6	uH = 1.60, d/s = -0.3, h = 0.35
0	1	23.1 22.2	1125	179.87	182.47	-0.08	22.12	0.28	
0	1	24.2	1150 1180	179.92	183.69		1172	6	
0	1	28.7	1240 1280	178.79	183.56		1273	6	
0	1	33.3	1380 1400	183.32	185.57	-5	1375	8	
0	1	37.0	1450 1500	182.04	187.45		1456	8	

40) ta + 5mag = 4fo + 5CO2 + H2O (Greenwood, 1967)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.40	2.0	540	562.57		-7	533	4	3 (563.93 <-> 572.63)
0	0.35	2.0	550		571.18		529	4	cH = 558.10 (sd 1.01) 2
0	0.75	2.0	560	563.61		-9	551	4	too low
0	0.73	2.0	586		579.20		550	4	uH = 3.11, d/s = 1.1, h = 0.01
0	0.51	2.0	560		570.17		540	4	

41) 2wo + 2mont = di + merw (Yoder, 1968)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	6.0 6.7	740	24.97	26.20		6.04	0.27	1 (25.09 <-> 26.03)
0	-	6.2 7.0	700	24.84	26.25		6.32	0.27	cH = 25.04 (sd 0.24)
0	-	6.5 7.3	650	24.75	26.16		6.67	0.27	too low but OK
									uH = 0.24, d/s = 2.5, h = 0.46

## CaO-MgO-SiO<sub>2</sub>

42) **wo + mont = ak** (Yoder, 1968)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.0	675 700	20.19	20.67	4	704	10	3 (20.52 <-> 20.79)
0	-	3.0	705 720	20.52	20.81		717	10	cH = 20.75 (sd 0.09)
0	-	5.0	720 750	20.56	21.13		730	10	within bracket
0	-	6.0	720 750	20.43	21.00		737	10	uH = 0.10, d/s = 0.6, h = 0.82

43) **di + merw = 2ak** (Yoder, 1968)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	7.5	780	14.64			850	20	3 (15.73 <-> 16.55)
0	-	7.0	810		16.43	1	811	18	cH = 16.45 (sd 0.24)
0	-	9.0	950 980	15.97	16.73		969	20	within bracket
0	-	10.0	1020 1050	15.73	16.50		1048	20	uH = 0.35, d/s = 0.7, h = 0.42

44) **di + 3mont = fo + 2ak** (Walter, 1963; Yoder, 1968)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.2	860 875	56.44	57.10		873	8	3 (56.77 <-> 57.46)
0	-	0.4	880 895	57.16	57.81	-4	876	8	cH = 56.99 (sd 0.17)
0	-	2.0	890 910	56.32	57.20		905	8	within bracket
0	-	5.0	950 975	56.54	57.63		960	8	uH = 0.25, d/s = -0.4, h = 0.89
0	-	10.0	1060 1090	57.29	58.61	-7	1053	8	

45) **2di + ta = tr** (Jenkins, Holland & Clare, 1991)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.16	-	27.0 24.0	650	-8.53	-6.91		25.52	0.64	3 (-8.18 <-> -7.41)
-0.16	-	26.5 26.0	700	-8.10	-7.83	-0.18	25.82	0.63	cH = -7.73 (sd 0.17)
-0.16	-	26.0 25.0	725	-7.75	-7.20		25.96	0.62	within bracket
-0.16	-	27.0 26.0	750	-8.22	-7.66		26.11	0.62	uH = 0.33, d/s = -0.1, h = 0.60

46) **di + 2mag = en + dol** (Brey et al., 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.01	-	23.0 20.0	850	9.76	10.91		20.03	2.92	3 (9.59 <-> 11.16)
0.05	-	28.5 25.5	970	9.83	10.92		25.55	3.11	cH = 10.90 (sd 0.56) 3
0.12	-	35.5 33.5	1100	9.92	10.59	-0.92	32.58	3.38	within bracket
0.15	-	41.5 39.5	1200	10.37	11.00		39.80	3.69	uH = 0.67, d/s = 0.1, h = 0.35
0.18	-	49.5 47.5	1300	10.46	11.03		47.95	4.09	

47) **spu + 2mont = 2merw + cc** (Walter, 1965)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.3	812 824	54.49	55.05	6	830	12	2 (54.81 <-> 55.39)
0	-	1.0	800 820	55.16	56.08		804	12	cH = 55.33 (sd 0.25)
									within bracket
									uH = 0.23, d/s = -0.2, h = 0.93

48) **2tr = 3en + 4di + 2q + 2H<sub>2</sub>O** (Yin & Greenwood, 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.1	655 675	228.76	233.45		674	4	3 (231.51 <-> 234.29)
0	0	0.2	725 745	231.33	235.65		733	4	cH = 233.12 (sd 0.36)
0	0	0.3	755 775	232.93	237.11		756	4	within bracket
0	0	0.8	800 820	231.08	234.87		811	4	uH = 0.99, d/s = -0.4, h = 0.17
0	0	1.4	820 840	228.68	232.19	5	845	4	

\* **2tr = 3en + 4di + 2q + 2H<sub>2</sub>O** (Boyd, 1959)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.6	795 820	233.71	238.63	-3	792	4	** NOT USED **
0	0	1.0	835 850	234.98	237.75	-10	825	4	cH = 233.12 (sd 0.36)
0	0	1.5	840 870	231.50	236.73		849	4	
0	0	2.0	860 880	232.21	235.56		865	4	

49)  $2tr = 3en + 4di + 2q + 2H_2O$  (Jenkins, Holland & Clare, 1991)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.5	840 860	231.50	234.99		849	4	3 (232.88 <-> 234.91)
0	0	3.0	880	232.12			886	4	cH = 233.12 (sd 0.36)
0	0	2.9	888		233.65		885	4	within bracket
0	0	5.0	914 930	234.17	236.55	-7	907	4	uH = 0.78, d/s = -0.3, h = 0.24
0	0	7.1	916 929	233.31	235.16	-1	915	6	

50)  $2tr + 2fo = 5en + 4di + 2H_2O$  (Jenkins, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.09	0	5.0	820 840	216.51	219.36		831	6	3 (214.97 <-> 218.25)
0.09	0	8.0	790 810	214.73	217.38	5	815	6	cH = 218.06 (sd 0.39)
0.09	0	10.0	770 790	214.65	217.22	7	797	6	within bracket
0.09	0	20.0	640 660	216.09	218.39		657	8	uH = 1.39, d/s = 0.3, h = 0.19

\*  $dol = cc + per + CO_2$  (Goldsmith, 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.14	1	9.0	1125 1140	118.23	119.30	36	1176	12	** NOT USED **
-0.14	1	9.5	1125 1150	117.04	118.82	43	1193	14	cH = 121.86 (sd 0.46)
-0.14	1	10.5	1050	109.36			1227	14	
-0.14	1	11.0	1180		117.55	63	1243	14	

\*  $dol = cc + per + CO_2$  (Harker & Tuttle, 1955)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.12	1	0.3	700 800	121.48	132.75		703	8	** NOT USED **
-0.12	1	0.7	780 820	123.97	128.16	-20	760	8	cH = 121.86 (sd 0.46)
-0.13	1	1.0	800 850	122.21	127.24	-3	797	10	
-0.13	1	2.8	900 950	120.30	124.75		918	10	

51)  $dol + 2q = di + 2CO_2$  (Slaughter et al., 75; Eggert & Kerrick, 1981; Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.95	2.0	505 525	156.20	159.63		508	6	3 (156.35 <-> 158.86)
0	0.73	6.0	610 630	156.32	159.37		613	6	cH = 156.76 (sd 0.48) 2
0	0.60	5.0	565 585	155.27	158.50		574	6	within bracket
									uH = 0.90, d/s = 1.2, h = 0.07

52)  $dol + 2q = di + 2CO_2$  (Eggler et al., 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	28.0	970 1025	152.29	158.03		1013	10	1 (152.91 <-> 157.40)
									cH = 156.76 (sd 0.48) 2
									within bracket
									uH = 0.92, d/s = 3.1, h = 0.01

\*  $dol + 2q = di + 2CO_2$  (Luth, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	35.0	1100 1150	156.58	161.25		1102	10	** NOT USED **
0	1	40.0	1150 1200	155.57	159.97		1163	10	cH = 156.76 (sd 0.48)
0	1	50.0	1300 1350	158.15	162.09	-17	1283	12	
0	1	60.0	1500 1550	163.92	167.36	-101	1399	14	

53)  $di + 3dol = 2fo + 4cc + 2CO_2$  (Kase & Metz, 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.33	0.90	3.0	623 653	207.27	213.48	9	662	12	3 (209.30 <-> 212.88)
-0.38	0.90	5.0	700 720	208.51	212.41	15	735	14	cH = 215.34 (sd 1.33) 2
-0.47	0.90	10.0	850 870	209.90	213.46	11	881	16	too high but OK
									uH = 1.43, d/s = 0.9, h = 0.25

54) 2dol + ta + 4q = tr + 4CO2 (Eggert & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.22	6.0	540 560	309.91	317.29	-11	529	6	2 (309.20 <-> 315.04)
0	0.21	6.0	530 550	306.88	314.33	-3	527	6	cH = 305.80 (sd 0.98) 2
									too low
									uH = 2.09, d/s = 1.1, h = 0.04

55) di + cc = ak + CO2 (Walter, 1963)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.05	1	0.5	895 905	151.97	153.12	-14	881	4	2 (151.59 <-> 153.10)
0.05	1	0.7	920 930	151.61	152.73	-11	909	4	cH = 150.36 (sd 0.25)
									too low
									uH = 0.64, d/s = 0.6, h = 0.19

56) ak + fo + cc = 3mont + CO2 (Walter, 1963)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.05	1	0.5	885 905	93.52	94.95	-2	883	8	2 (92.93 <-> 94.19)
0.05	1	0.7	910 930	92.24	93.60		927	8	cH = 93.37 (sd 0.28)
									within bracket
									uH = 0.45, d/s = 0.1, h = 0.30

57) fo + di + 2cc = 3mont + 2CO2 (Walter, 1963)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.10	1	0.5	885 905	244.33	248.07	-3	882	6	1 (244.55 <-> 247.85)
									cH = 243.73 (sd 0.51)
									too low but OK
									uH = 1.10, d/s = 1.7, h = 0.07

58) 5dol + 4ta = 6fo + 5di + 4H2O + 10CO2 (Skippen, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.75	1.0	500 540	1242.03	1296.56		516	4	1 (1252.32 <-> 1273.66)
0	0.75	2.0	550 570	1250.34	1275.64		561	4	cH = 1264.30 (sd 2.62) 2
									within bracket
									uH = 6.60, d/s = 1.9, h = 0.01

59) ta + 3cc + 2q = 3di + H2O + 3CO2 (Skippen, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.60	2.0	480 515	307.07	318.61		493	6	1 (308.31 <-> 317.37)
									cH = 311.33 (sd 1.02) 2
									within bracket
									uH = 1.71, d/s = 3.4, h = 0.01

60) 5dol + 8q + H2O = tr + 3cc + 7CO2 (Slaughter et al., 1975; Eggert & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.12	0.85	2.0	474 494	459.00	470.01		484	8	3 (464.69 <-> 473.73)
-0.22	0.66	6.0	590 610	462.95	472.87		594	8	cH = 464.75 (sd 2.06) 2
-0.19	0.21	6.0	540 560	470.27	482.37	-9	531	6	within bracket
-0.19	0.21	6.0	530 550	464.19	476.33		531	6	uH = 3.23, d/s = -0.0, h = 0.14

61) 5ta + 6cc + 4q = 3tr + 6CO2 + 2H2O (Slaughter et al., 1975;)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.50	2.0	425 465	586.60	613.78		444	6	1 (589.32 <-> 611.06)
									cH = 599.49 (sd 2.13) 2
									within bracket
									uH = 3.51, d/s = 3.9, h = 0.01

62)  $3\text{dol} + 4\text{q} + \text{H}_2\text{O} = \text{ta} + 3\text{cc} + 3\text{CO}_2$  (Eggert & Kerrick, 1981; Metz & Puhon, 1971; Gordon & Greenwood)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.15	0.50	3.0	485	505	158.74	163.03		486	12	3 (158.25 <-> 161.83)
-0.19	0.50	5.0	550	570	157.30	161.30		558	12	cH = 158.95 (sd 1.26) 2
-0.19	0.25	6.0	540	560	157.56	162.10		546	12	within bracket
-0.09	0.45	2.0	450		161.46		-11	439	10	uH = 1.28, d/s = -0.1, h = 0.25
-0.12	0.57	2.0		472		163.07		453	12	
-0.12	0.79	2.0	470		154.60			492	12	
-0.15	0.76	2.0		497		161.62		484	12	
-0.15	0.93	2.0	519		154.80			542	14	

63)  $\text{tr} + 3\text{cc} + 2\text{q} = 5\text{di} + 3\text{CO}_2 + \text{H}_2\text{O}$  (Slaughter et al., 1975)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.50	1.0	489	499	322.97	326.52	-11	478	6	2 (321.94 <-> 326.22)
0	0.90	1.0	476	496	318.12	325.18		479	6	cH = 319.06 (sd 1.03) 2
										too low
										uH = 1.82, d/s = 0.6, h = 0.07

64)  $\text{tr} + 11\text{dol} = 8\text{fo} + 13\text{cc} + 9\text{CO}_2 + \text{H}_2\text{O}$  (Metz, 1976)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.67	0.50	1.0	525	545	1007.68	1030.28		539	8	3 (1007.41 <-> 1024.20)
-0.80	0.50	3.0	610	630	1005.48	1025.68		628	10	cH = 1023.65 (sd 4.69) 2
-1.08	0.50	5.0	670	690	1003.97	1024.23		691	10	within bracket
										uH = 6.01, d/s = 1.4, h = 0.15

65)  $3\text{tr} + 5\text{cc} = 11\text{di} + 2\text{fo} + 5\text{CO}_2 + 3\text{H}_2\text{O}$  (Chernosky & Berman, 1986)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.45	1.0	528	548	692.18	706.59		542	6	1 (693.35 <-> 705.42)
										cH = 702.24 (sd 1.85) 2
										within bracket
										uH = 3.69, d/s = 2.0, h = 0.02

## Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

66) **ky = and** (Holdaway, 1971; Newton, 1966a; Richardson et al., 1969; Bohlen et al 1991)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	2.4	377 409	4.24	4.54		390	12	3 (4.22 <-> 4.42)
0	-	3.6	447 499	3.99	4.47		487	12	cH = 4.36 (sd 0.05)
0	-	4.8	557 590	4.10	4.40		585	12	within bracket
0	-	7.0 5.6	700	3.75	4.79		6.18	0.15	uH = 0.07, d/s = 1.1, h = 0.50
0	-	7.5 5.6	750	3.82	5.23		6.77	0.15	
0	-	7.9 6.5	800	3.96	5.00		7.36	0.15	
0	-	8.5 6.9	800	3.51	4.70		7.36	0.15	
0	-	6.8 6.0	700	3.86	4.49		6.18	0.15	
0	-	7.9 7.2	825	4.18	4.66		7.66	0.15	
0	-	8.2	800	3.73			871	12	

67) **ky = sill** (Newton, 1966b; Richardson et al., 1969; Holdaway, 1971; Bohlen et al., 1991)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	7.0 5.5	600	6.60	7.43		5.85	0.23	3 (7.27 <-> 7.57)
0	-	8.8 7.0	700	6.81	7.80		8.02	0.23	cH = 7.24 (sd 0.06)
0	-	10.3 9.0	800	7.19	7.90		10.22	0.23	too low but OK
0	-	12.2 11.3	900	7.38	7.86	0.26	12.46	0.23	uH = 0.11, d/s = 0.3, h = 0.24
0	-	15.1 13.9	1000	7.05	7.68		14.74	0.24	
0	-	9.5 7.5	750	7.03	8.12		9.11	0.23	
0	-	9.0 7.2	750	7.30	8.28	0.11	9.11	0.23	
0	-	8.2	685	6.96			708	10	
0	-	7.0	710		7.92		653	10	
0	-	9.2	740	7.07			754	10	
0	-	8.8	785		7.83		736	10	
0	-	10.2	790	7.13			799	10	
0	-	9.8	835		7.88		781	10	
0	-	28.0 26.5	1500	6.80	7.53		27.10	0.26	
0	-	23.5	1300	6.45			1362	10	

68) **and = sill** (Holdaway, 1971; Bowman 1975; Kerrick & Heninger, 1984)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.8	571 663	2.69	2.94		642	28	1 (2.81 <-> 2.89)
0	-	3.6	491 527	2.80	2.90		520	28	cH = 2.88 (sd 0.04)
0	-	3.0	497	2.71			559	28	within bracket
0	-	4.3	506		2.97		475	26	uH = 0.02, d/s = 2.6, h = 0.85
0	-	1.2 2.5	615	2.69	2.94		2.19	0.38	
0	-	0.5	669 806	2.70	3.06		738	30	
0	-	3.0	607		3.01		559	28	
0	-	0.0	805		2.96		776	30	

\* **and = sill** (Richardson et al., 1969)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	2.0	750 800	3.21	3.35	-122	628	28	** NOT USED **
0	-	3.0	650 750	3.13	3.41	-91	559	28	cH = 2.88 (sd 0.04)
0	-	4.0	650	3.32		-156	494	26	

69) **ky = cor + q** (Harlov & Newton, 1993)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	5.5 4.8	700	6.90	7.24		5.17	0.30	2 (6.88 <-> 7.09)
0	-	8.0 7.5	800	6.84	7.07		7.53	0.31	cH = 7.06 (sd 0.06)
									within bracket
									uH = 0.08, d/s = 1.0, h = 0.33

70) **cor + q = and** (Harlov & Newton, 1993)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	8.0 7.5	700	-2.76	-2.61		7.79	0.19	1 (-2.76 <-> -2.62)
									cH = -2.70 (sd 0.04) 0.5
									within bracket
									uH = 0.05, d/s = 1.6, h = 0.84



71) 2dsp = cor + H2O (Haas, 1972; Hemley et al., 1980; Grevel et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	382 406	82.56	84.27	-11	371	4	5 (80.97 <-> 82.31)
0	0	1.8	385 410	81.77	83.54		385	4	cH = 81.80 (sd 0.18)
0	0	2.4	392 415	81.46	83.11		397	4	within bracket
0	0	3.5	410 430	81.51	83.02		414	4	uH = 0.37, d/s = -1.8, h = 0.56
0	0	4.8	415 440	80.62	82.47		431	4	
0	0	7.0	450 470	81.28	82.73		457	4	
0	0	14.5	500 530	79.60	81.63	3	533	6	
0	0	24.0	575 600	79.60	81.20	9	609	6	
0	0	28.5	625 650	80.81	82.37		641	6	
0	0	38.0	670 700	80.03	81.84		699	6	
0	0	47.5	700 740	78.92	81.28	9	749	8	

72) 2dsp = cor + H2O (Vidal et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.05	0	25.0	595 615	80.80	82.08		611	6	1 (80.85 <-> 82.03)
-0.05	0	28.0	615 650	80.77	82.97		631	6	cH = 81.80 (sd 0.18)
									within bracket
									uH = 0.42, d/s = 1.5, h = 0.10

73) prl + 6dsp = 4and + 4H2O (Haas & Holdaway, 1973; Hemley et al., 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	325 349	309.46	316.62		343	4	3 (309.49 <-> 313.67)
0	0	2.4	340 400	305.82	321.97		373	4	cH = 314.94 (sd 0.72) 2
0	0	3.5	365 395	307.05	314.74	1	396	4	too high but OK
0	0	4.8	395 415	308.32	313.70	4	419	4	uH = 1.50, d/s = 1.4, h = 0.06
0	0	7.0	435 455	309.29	314.93		455	6	

74) 2dsp + 4q = prl (Theye et al., 1997)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	25.0	500 535	1.31	1.48		533	26	2 (1.42 <-> 1.56)
0	-	23.0	500 540	1.49	1.69	-5	495	24	cH = 1.47 (sd 0.06)
									within bracket
									uH = 0.05, d/s = -0.2, h = 0.97

75) 2dsp + 4coe = prl (Theye et al., 1997)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	28.3 26.0	550	-20.67	-18.63		27.53	0.47	1 (-20.49 <-> -18.82)
									cH = -19.99 (sd 0.21)
									within bracket
									uH = 0.48, d/s = 2.1, h = 0.05

76) prl = cor + 4q + H2O (Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	3.0	400 460	78.54	82.86		425	6	1 (80.12 <-> 82.20)
0	0	5.0	440 500	79.48	83.69		452	6	cH = 80.33 (sd 0.18)
0	0	7.0	460 520	79.26	83.33		476	6	within bracket
0	0	10.0	500 540	79.85	82.47		507	6	uH = 0.35, d/s = 3.7, h = 0.05

77) prl = and + 3q + H2O (Hemley et al., 1980; Kerrick, 1968)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	354 378	77.52	79.15		356	4	3 (78.41 <-> 79.29)
0	0	1.8	395 425	78.96	81.08	-22	373	4	cH = 77.63 (sd 0.19)
0	0	3.9	415 445	77.47	79.57		417	4	too low
									uH = 0.32, d/s = 0.3, h = 0.14

78) prl = and + 3q + H2O (Haas & Holdaway, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	3.5	390 415	76.38	77.97		410	4	1 (76.43 <-> 77.38)
0	0	4.8	410 430	76.07	77.43	3	433	6	cH = 77.63 (sd 0.19) 2
0	0	7.0	450 470	76.36	77.70		469	6	too high but OK
									uH = 0.33, d/s = 1.6, h = 0.06

79) kao + 2q = prl + H2O (McPhail unpub; Hemley et al., 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	261 285	59.88	61.25	3	288	6	2 (60.91 <-> 61.70)
0	0	5.0	306 333	61.35	62.84		307	8	cH = 61.43 (sd 0.37)
									within bracket
									uH = 0.28, d/s = -0.2, h = 0.65

80) 2kao = 2dsp + prl + 2H2O (Hemley et al., 1980)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	288 312	120.56	123.29		295	8	1 (120.84 <-> 123.02)
									cH = 121.38 (sd 0.73)
									within bracket
									uH = 0.57, d/s = 2.4, h = 0.35

81) tpz = ky + H2O (Wunder et al. 93)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	55.0 50.0	700	68.04	70.09		50.06	3.18	2 (69.33 <-> 70.80)
0	0	90.0 85.0	1000	70.04	71.68		89.93	4.14	cH = 70.06 (sd 0.67)
									within bracket
									uH = 0.56, d/s = 0.0, h = 1.00

## CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

82) **cz = zo** (Holland, unpub)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	6.0	325 375	-0.79	-0.44		373	78	1 (-0.56 <-> -0.45)
0	-	15.0	350 500	-0.57	0.76		369	98	cH = -0.46 (sd 0.31) 2 within bracket uH = 0.03, d/s = 1.9, h = 0.82

83) **gr + 2ky + q = 3an** (Koziol & Newton, 1987; Goldsmith, 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	25.3 24.9	1150	38.83	41.24		24.98	0.20	3 (36.62 <-> 43.51)
0	-	23.2 22.8	1050	37.43	39.86	-0.15	22.65	0.20	cH = 40.75 (sd 0.61)
0	-	24.3 23.2	1100	37.81	44.46		23.81	0.20	within bracket
0	-	22.3 21.3	1000	35.87	41.98		21.50	0.20	uH = 2.92, d/s = 0.0, h = 0.26
0	-	20.3 18.8	900	34.08	43.33		19.22	0.20	
0	-	21.1 20.3	950	36.19	41.10		20.36	0.20	
0	-	24.0 22.0	1100	39.62	51.74		23.81	0.20	
0	-	26.0 24.0	1150	34.63	46.66		24.98	0.20	
0	-	26.7 25.8	1200	37.52	42.90		26.16	0.20	
0	-	28.2 27.1	1250	35.68	42.21		27.35	0.20	
0	-	27.0 25.0	1200	35.72	47.69		26.16	0.20	
0	-	28.0 26.0	1250	36.86	48.77		27.35	0.20	
0	-	29.0 27.0	1300	38.05	49.91		28.54	0.20	

\* **gr + 2ky + q = 3an** (Gasparik, 1984; Hays, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	26.4 25.3	1200	39.31	45.89		26.16	0.20	** NOT USED **
0	-	28.2 27.3	1300	42.79	48.13	0.34	28.54	0.20	cH = 40.75 (sd 0.61)
0	-	27.0 23.0	1200	35.72	59.71		26.16	0.20	
0	-	29.0 28.0	1300	38.05	43.97		28.54	0.20	
0	-	32.0 30.0	1400	34.78	46.49		30.98	0.21	

84) **gr + q = an + 2wo** (Huckenholz et al., 1975; Newton, 1966; Hays, 1967; Windom & Boettcher, 1976)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	2.0	565 585	52.45	53.88		578	8	3 (52.92 <-> 54.06)
0	-	3.0	615 635	52.81	54.23		623	8	cH = 53.37 (sd 0.29)
0	-	4.0	665 685	53.16	54.57		668	8	within bracket
0	-	4.7	695 725	53.06	55.17		699	8	uH = 0.41, d/s = 0.9, h = 0.72
0	-	6.3 5.4	750	51.88	54.72		5.83	0.18	
0	-	14.5 13.5	1100	51.23	54.31		13.80	0.19	
0	-	16.1 11.6	1100	46.32	60.20		13.80	0.19	
0	-	17.0 15.3	1200	50.77	55.97		16.15	0.19	

85) **gr + cor = geh + an** (Boettcher, 1970; Huckenholz et al., 1975)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.0	760 780	98.92	100.98		761	14	3 (100.22 <-> 101.90)
0	-	5.0	930 950	100.08	102.13	-11	919	16	cH = 98.99 (sd 0.77) 2
0	-	6.0	975 995	100.65	102.70	-16	959	16	too low but OK uH = 0.61, d/s = 0.3, h = 0.41

86) **2gr = 3wo + geh + an** (Huckenholz et al., 1975; Hays, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.0	880 900	162.83	165.88		899	12	3 (162.25 <-> 164.99)
0	-	2.0	920 940	162.75	165.79		940	12	cH = 165.73 (sd 0.86) 2
0	-	3.0	960 985	162.69	166.49		980	12	too high but OK
0	-	7.5	1120 1150	159.58	164.15	10	1160	12	uH = 0.98, d/s = 0.7, h = 0.28
0	-	10.2	1240	161.57			1267	12	
0	-	8.8	1210		165.43	2	1212	12	
0	-	10.0 7.5	1200	156.68	171.78		8.50	0.29	
0	-	11.0 9.0	1250	158.30	170.33		9.76	0.29	

87)  $gr + 2cor = 3cats$  (Gasparik, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	12.8 11.3	1170	71.85	73.97		11.58	0.53	3 (72.90 <-> 74.24)
0	-	15.5 14.4	1230	72.25	73.78		14.55	0.54	cH = 73.57 (sd 0.37)
0	-	17.0 15.9	1270	72.96	74.48		16.56	0.54	within bracket
0	-	18.1 16.9	1300	73.54	75.20		18.08	0.54	uH = 0.57, d/s = 0.2, h = 0.97
0	-	23.7 22.5	1400	72.97	74.58		23.25	0.56	
0	-	29.3 28.2	1500	72.64	74.07		28.58	0.57	

88)  $gr + 3ky = 3an + cor$  (Gasparik, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	28.2 27.4	1300	46.02	51.11		27.92	0.19	2 (44.31 <-> 52.82)
0	-	30.7 29.8	1400	45.65	51.31		30.36	0.20	cH = 47.81 (sd 0.61)
									within bracket
									uH = 3.61, d/s = 0.7, h = 0.04

89)  $gr + 3cats = 2an + 2geh$  (Hays, 1967)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	14.9 13.9	1300	119.15	125.62		14.09	0.49	1 (119.49 <-> 125.28)
									cH = 124.40 (sd 1.55) 2
									within bracket
									uH = 1.98, d/s = 1.6, h = 0.06

90)  $3cats = an + geh + cor$  (Hays, 1967)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	13.9 10.9	1200	19.83	27.47		11.71	0.67	1 (24.70 <-> 26.70)
0	-	13.0 11.8	1250	23.76	26.81		12.35	0.67	cH = 25.41 (sd 0.83) 2
0	-	14.0 12.0	1350	24.48	29.55		13.63	0.68	within bracket
0	-	14.6 13.0	1400	24.59	28.62		14.27	0.68	uH = 0.69, d/s = 1.6, h = 0.18

91)  $gr + 3ky = 3an + cor$  (Gasparik, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	28.3 27.3	1300	45.39	51.74		27.92	0.19	2 (44.31 <-> 52.82)
0	-	30.8 29.7	1400	45.02	51.94		30.36	0.20	cH = 47.81 (sd 0.61)
									within bracket
									uH = 3.61, d/s = 0.9, h = 0.03

92)  $3an + cc = me$  (Baker & Newton, 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.5	847 860	63.95	64.67		854	10	3 (63.98 <-> 64.70)
0	-	3.6	848	63.85			857	10	cH = 64.34 (sd 0.30)
0	-	3.2	865		64.82		856	10	within bracket
0	-	6.7	853	63.90			861	10	uH = 0.28, d/s = 1.2, h = 0.99
0	-	7.2	873		64.96		862	10	
0	-	15.0	865 880	64.00	64.81		871	10	

\*  $3an + cc = me$  (Goldsmith & Newton, 1977)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	1.0	850 900	64.15	66.92		853	10	** NOT USED **
0	-	5.0	850 900	63.85	66.61		859	10	cH = 64.34 (sd 0.30)
0	-	8.0	850 900	63.64	66.39		863	10	
0	-	10.0	850 875	63.50	64.87		865	10	
0	-	15.0	850 900	63.18	65.90		871	10	

93) gr + cc + 2ky + q = me (Baker & Newton, 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	19.7	900	103.38			909	6	3 (101.78 <-> 108.79)
0	-	23.0 22.1	1000	102.38	107.93		22.56	0.21	cH = 105.09 (sd 0.67)
0	-	26.5 26.0	1100	100.36	103.40	-0.28	25.72	0.22	within bracket
0	-	29.4	1200	102.26			1215	6	uH = 2.97, d/s = 0.0, h = 0.06
0	-	27.5	1190		111.77		1156	6	
0	-	26.6	1145		108.47		1128	6	

94) 4zo + q = 5an + gr + 2H2O (Boettcher, 1970; Newton, 1966; Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	570 610	207.80	216.50		580	4	3 (207.48 <-> 211.08)
0	0	5.3	630 660	207.50	213.89		642	4	cH = 210.06 (sd 0.48)
0	0	2.0	485 535	210.18	221.49	-1	484	4	within bracket
0	0	4.7	600	207.13			614	4	uH = 1.53, d/s = -0.7, h = 0.26
0	0	6.0 5.5	650	204.76	209.75	-0.03	5.47	0.10	
0	0	7.5 6.8	720	204.70	211.53		6.95	0.10	
0	0	2.0	480 510	209.05	215.83		484	4	
0	0	5.1	610 640	205.23	211.65		633	4	
0	0	6.0	660 670	206.87	208.98	5	675	4	
0	0	8.0	740 760	204.00	208.10	10	770	4	

95) 4zo + q = 5an + gr + 2H2O (Newton, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.6	600 640	208.15	216.76		609	4	3 (207.16 <-> 211.73)
0	0	6.0	650 700	204.76	215.29		675	4	cH = 210.06 (sd 0.48)
0	0	8.0	740 770	204.00	210.14		770	4	within bracket
									uH = 1.64, d/s = 0.6, h = 0.05

96) 6zo = 6an + 2gr + cor + 3H2O (Boettcher 1970; Newton 1965; Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	3.0	620 665	299.04	311.26		630	6	3 (301.07 <-> 305.11)
0	0	2.0	570 585	299.29	303.52		579	6	cH = 301.78 (sd 0.78)
0	0	4.1	670 700	297.73	305.64		685	6	within bracket
0	0	4.6	700 730	299.11	306.90		710	6	uH = 1.71, d/s = 0.1, h = 0.61
0	0	5.6	765 795	303.06	310.62	-5	760	6	
0	0	6.1	785 815	301.84	309.32		785	6	
0	0	6.8	815 845	300.68	308.04		819	6	
0	0	2.0	560 590	296.48	304.93		579	6	
0	0	4.0	680 690	301.69	304.33		680	6	
0	0	8.0	870 890	299.61	304.39		879	6	

97) 2cz + ky + q = 4an + H2O (Jenkins et al., 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	7.5 7.1	550	120.54	123.77	-0.09	7.01	0.18	1 (120.29 <-> 124.03)
									cH = 124.49 (sd 0.71)
									too high but OK
									uH = 1.57, d/s = 1.0, h = 0.11

98) 4cz + q = 5an + gr + 2H2O (Liou, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
6.19	0	3.0	670 694	208.24	214.46		670	10	1 (208.74 <-> 213.96)
									cH = 208.23 (sd 1.30) 2
									too low but OK
									uH = 1.61, d/s = 1.9, h = 0.05

99) 4cz + q = 5an + gr + 2H2O (Holdaway, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
6.19	0	3.0	690 710	213.42	218.66	-20	670	10	1 (213.68 <-> 218.40)
									cH = 208.23 (sd 1.30) 2
									too low
									uH = 1.63, d/s = 1.6, h = 0.06

100) 2zo + ky + q = 4an + H2O (Goldsmith, 1981; Jenkins et al., 1983; Johannes, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0 3.0	400	118.99	127.28		3.22	0.09	3 (122.17 <-> 126.43)
0	0	5.0 4.2	450	119.70	126.26		4.30	0.10	cH = 125.41 (sd 0.39)
0	0	6.0	510 530	122.26	125.81		528	4	within bracket
0	0	5.0	450 490	119.70	126.84		482	4	uH = 1.81, d/s = 0.3, h = 0.20
0	0	7.8 7.0	580	120.16	126.57		7.14	0.10	
0	0	7.0	550 580	121.28	126.57		573	4	
0	0	8.0	570 625	116.80	126.47		619	4	
0	0	9.0	650 675	122.89	127.25		664	4	
0	0	10.0	705 725	124.57	128.02		710	4	
0	0	10.3	695 725	120.49	125.67		723	4	

101) 2zo + sill + q = 4an + H2O (Newton, 1966; Newton & Kennedy, 1963)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	7.5 7.0	550	111.54	115.27	-0.39	6.61	0.11	3 (113.86 <-> 117.75)
0	0	9.2 8.6	650	115.32	119.74		8.81	0.11	cH = 118.17 (sd 0.40)
0	0	9.3 7.7	620	109.71	121.53		8.15	0.11	too high but OK
0	0	10.0	670 730	112.71	122.37		704	4	uH = 1.45, d/s = -0.0, h = 0.08

102) ma = an + cor + H2O (Chatterjee, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	470 500	90.14	92.71		477	4	3 (90.46 <-> 91.43)
0	0	2.0	500 520	90.24	91.85		506	4	cH = 90.71 (sd 0.17)
0	0	4.0	560 570	90.87	91.63	-2	558	4	within bracket
0	0	6.0	600 610	90.31	91.03		606	4	uH = 0.41, d/s = 0.2, h = 0.31
0	0	7.0	620 640	90.10	91.53		628	4	

\* ma = an + cor + H2O (Storre & Nitsch, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	3.0	510 530	88.96	90.51	3	533	4	** NOT USED **
0	0	5.0	570 590	89.82	91.30		582	4	cH = 90.71 (sd 0.17)
0	0	7.0	620 660	90.10	92.95		628	4	

\* ma + q = an + and + H2O (Storre & Nitsch, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	490 540	84.25	87.98		540	4	** NOT USED **
0	0	5.0	515 560	84.09	87.38	9	569	4	cH = 88.01 (sd 0.17)

\* ma + q = an + ky + H2O (Storre & Nitsch, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	5.0	530 570	81.48	84.04		564	6	** NOT USED **
0	0	7.0	580 600	82.24	83.47	3	603	6	cH = 83.65 (sd 0.16)
0	0	9.0	640 660	83.70	84.89	-1	639	6	

103) 4ma + 3q = 2zo + 5ky + 3H2O (Jenkins, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	9.0 10.0	500	204.50	208.58	0.15	10.15	0.29	3 (208.16 <-> 210.28)
0	0	8.4 10.0	550	205.48	211.77		9.36	0.30	cH = 209.19 (sd 0.58)
0	0	8.4 9.0	600	208.82	211.06		8.50	0.33	within bracket
0	0	7.7 8.3	650	209.66	211.76	-0.14	7.56	0.36	uH = 0.76, d/s = -0.7, h = 0.67

\*  $ma + q = an + and + H_2O$  (Nitsch et al., 1981)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	440	460	84.76	86.33	21	481	4	** NOT USED **
0	0	4.0	510	520	85.74	86.49	20	540	4	cH = 88.01 (sd 0.17)
0	0	5.0	560	570	87.38	88.11		569	4	

\*  $ma + q = an + ky + H_2O$  (Nitsch et al., 1981)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	6.0	575	585	83.10	83.73		584	6	** NOT USED **
0	0	7.0	590	600	82.86	83.47	3	603	6	cH = 83.65 (sd 0.16)

104)  $4ma = 2zo + 2ky + 3cor + 3H_2O$  (Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	12.0	540		226.86			580	14	1 (227.19 <-> 229.95)
0	0	13.0		550		230.74		546	14	cH = 230.37 (sd 0.59)
0	0	10.0	600	640	226.63	230.29	1	641	14	too high but OK
										uH = 0.76, d/s = 2.3, h = 0.13

105)  $law = an + 2H_2O$  (Crawford & Fyfe, 1965)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	6.9	400	450	145.33	152.35		448	4	1 (148.91 <-> 151.96)
0	0	6.0 4.5	400		148.52	154.04		5.02	0.13	cH = 152.08 (sd 0.25)
0	0	5.5	375		147.25			413	2	too high but OK
										uH = 0.79, d/s = 2.4, h = 0.02

106)  $4law + 2q = 2zo + prl + 6H_2O$  (Nitsch, 1972)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	7.0	370	430	405.00	422.92		386	4	1 (406.22 <-> 421.69)
										cH = 409.65 (sd 0.95)
										within bracket
										uH = 1.76, d/s = 5.1, h = 0.01

\*  $12law = 6zo + 2ky + prl + 20H_2O$  (Nitsch, 1972)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	340	375	1379.92	1417.51	-4	336	4	** NOT USED **
0	0	7.0	390	430	1375.05	1416.17		391	4	cH = 1375.50 (sd 2.78)

107)  $5law = 2zo + ma + 2q + 8H_2O$  (Nitsch, 1974)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	325	355	553.34	567.37	-4	321	4	3 (550.03 <-> 557.31)
0	0	7.0	370	400	547.44	559.14		380	4	cH = 551.36 (sd 1.16)
0	0	10.0	415	445	541.75	555.17		437	6	within bracket
										uH = 2.61, d/s = 0.4, h = 0.12

108)  $2law + dsp = zo + ky + 4H_2O$  (Schmidt & Poli, 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	16.0	510	540	278.77	284.79		510	4	5 (277.17 <-> 280.93)
0	0	22.0	550	580	273.33	279.03		579	6	cH = 278.84 (sd 0.47)
0	0	28.5	630	660	275.39	280.73		649	6	within bracket
0	0	33.0	710	725	281.18	283.72	-14	696	6	uH = 1.38, d/s = -0.8, h = 0.16
0	0	36.0		740		281.01		727	6	

109) 4law = 2zo + ky + q + 7H2O (Schmidt & Poli, 1994; Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	16.0	510 550	478.67	492.43		522	6	3 (478.60 <-> 485.15)
0	0	22.0	580	475.98			602	6	cH = 482.93 (sd 0.92)
0	0	21.5	598		483.87		595	6	within bracket
0	0	19.0	545 577	477.16	487.80		562	6	uH = 2.35, d/s = 1.1, h = 0.06
0	0	14.0	480 550	477.57	502.19		495	6	

110) 4law = 2zo + ky + q + 7H2O (Newton & Kennedy, 1963)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	13.5	500		487.09		488	6	3 (480.99 <-> 486.69)
0	0	17.5	540 550	482.10	485.48		542	6	cH = 482.93 (sd 0.92)
0	0	21.5	590	481.29			595	6	within bracket
0	0	25.0	640 650	482.85	485.95		640	6	uH = 2.42, d/s = 0.5, h = 0.26
0	0	29.5	660 720	471.76	489.54		698	6	
0	0	33.5	730 760	477.82	486.33		748	8	

111) 4law = 2zo + ky + coe + 7H2O (Skrok et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	19.0	565 595	487.39	497.28		568	6	3 (483.47 <-> 490.78)
0	0	24.0	615 645	483.59	492.97		630	6	cH = 488.29 (sd 0.92)
0	0	28.5	670 705	483.89	494.30		685	6	within bracket
0	0	33.0	720 750	482.97	491.51		739	8	uH = 2.65, d/s = -0.8, h = 0.28
0	0	38.0	770 805	480.71	490.20		798	8	
0	0	43.0	820 855	478.75	487.82	2	857	8	
0	0	47.5	855 890	474.66	483.40	20	910	10	

\* pre = an + wo + H2O (Chatterjee et al., 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	410 430	89.76	91.59	23	453	4	** NOT USED **
0	0	1.0	430 460	90.11	92.77	12	472	4	cH = 93.82 (sd 0.19)
0	0	2.0	460 470	90.14	90.98	33	503	4	
0	0	4.0	500 520	88.87	90.47	42	562	4	
0	0	5.0	530 540	89.14	89.93	49	589	4	

112) 5pre = 2zo + 2gr + 3q + 4H2O (Connolly & Kerrick, 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	410 430	228.36	231.15		427	8	5 (229.66 <-> 231.65)
0	0	2.0	407 427	229.44	231.87		417	6	cH = 230.65 (sd 0.51)
0	0	4.0	380 400	232.57	233.78	-24	356	6	within bracket
									uH = 0.58, d/s = -1.2, h = 1.00

113) wrk = an + 2q + 2H2O (Liou, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	340 355	125.00	126.23	18	373	6	4 (127.17 <-> 128.34)
0	0	2.0	365 380	126.83	127.88		377	8	cH = 127.67 (sd 0.40) 2
0	0	3.0	365 390	126.95	128.56		376	8	within bracket
0	0	4.3	375 405	128.11	129.88	-7	368	8	uH = 0.35, d/s = -3.6, h = 0.52
0	0	5.0	380 400	128.78	129.85	-18	362	8	

114) lmt = an + 2q + 4H2O (Thompson, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	300 320	245.34	248.83		304	2	3 (243.54 <-> 245.74)
0	0	2.0	307 327	243.72	247.01		322	2	cH = 246.12 (sd 0.34) 2
0	0	4.0	328 348	242.53	245.53	4	352	2	too high but OK
0	0	6.0	337 357	240.45	243.24	22	379	4	uH = 0.79, d/s = -1.3, h = 0.05



115)  $lmt = wrk + 2H_2O$  (Liou, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	220 240	118.05	119.81		225	4	5 (118.11 <-> 119.38)
0	0	1.0	250 260	119.26	120.14	-9	241	4	cH = 118.45 (sd 0.40) 2
0	0	2.0	274 284	118.59	119.44	-2	272	4	within bracket
0	0	3.0	294 301	117.62	118.20	3	304	4	uH = 0.44, d/s = -4.3, h = 0.54
0	0	5.0	316 328	114.49	115.42	41	369	8	

116)  $law + 2q + 2H_2O = lmt$  (Liou, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	3.0 2.8	200	-93.06	-92.67	0.49	3.49	0.26	4 (-94.22 <-> -93.80)
0	0	3.5 3.0	250	-94.48	-93.54		3.27	0.28	cH = -94.04 (sd 0.27) 2
0	0	3.5 3.2	300	-95.04	-94.51	-0.28	2.92	0.31	within bracket
									uH = 0.13, d/s = -5.8, h = 0.85

117)  $law + 2q = wrk$  (Liou, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	3.2	312		23.92	7	319	12	3 (23.14 <-> 24.25)
0	-	3.5	305 333	22.16	24.09	5	338	12	cH = 24.41 (sd 0.40) 2
0	-	4.0	355 365	23.47	24.16	4	369	12	too high but OK
0	-	4.3	381	23.98			387	12	uH = 0.47, d/s = -0.1, h = 0.16

118)  $heu = lmt + 3q + 2H_2O$  (Cho et al., 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.5	160 190	113.27	115.38		178	12	1 (113.87 <-> 115.21)
0	0	2.0	160 190	113.70	115.77		172	12	cH = 114.54 (sd 1.32) 2
									within bracket
									uH = 0.35, d/s = 2.4, h = 1.00

119)  $stlb = lmt + 3q + 3H_2O$  (Liou, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	178		171.15	12	190	8	5 (171.50 <-> 173.34)
0	0	3.0	170 198	170.46	173.40		189	8	cH = 172.42 (sd 1.39) 2
0	0	4.0	175 205	171.28	174.39		186	8	within bracket
0	0	5.0	173 195	171.55	173.73		182	8	uH = 0.51, d/s = -0.4, h = 1.00

120)  $3cc + an + cor = 2geh + 3CO_2$  (Shmulovich, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	0.5	790 830	367.83	380.35		820	10	1 (372.47 <-> 377.60)
0	1	0.7	835 855	372.03	378.04		852	12	cH = 377.18 (sd 1.68) 2
									within bracket
									uH = 1.62, d/s = 1.9, h = 0.10

121)  $2cc + an = wo + geh + 2CO_2$  (Shmulovich, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	0.5	840 860	236.13	239.91	4	864	10	2 (236.02 <-> 238.84)
0	1	0.7	870 890	235.11	238.74	11	901	10	cH = 240.71 (sd 0.89) 2
									too high
									uH = 1.01, d/s = 1.3, h = 0.12

\*  $wo + cc + an = gr + CO_2$  (Hoschek, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.37	1.0	715	38.38		-37	678	28	** NOT USED **
0	0.30	1.0	735		40.24		631	26	cH = 37.49 (sd 0.34)
0	0.52	1.0	815	38.10		-33	782	36	
0	0.45	1.0	835		39.59		732	32	
0	0.13	4.0	715	40.00		-111	604	30	
0	0.10	4.0	735		42.24		549	26	
0	0.23	4.0	815	37.90		-30	785	48	
0	0.18	4.0	835		39.96		691	36	

\*  $an + cor + 3cc = 2geh + 3CO_2$  (Hoschek, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.31	1.0	765	367.08			796	10	** NOT USED **
0	0.27	1.0	785		376.61	2	787	10	cH = 377.18 (sd 1.68)
0	0.63	1.0	815	367.31			848	12	
0	0.56	1.0	835		376.23	3	838	10	

\*  $2an + 3cc = geh + gr + 3CO_2$  (Hoschek, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.42	1.0	790	266.73			844	10	** NOT USED **
0	0.34	1.0	810		275.70	11	821	10	cH = 278.20 (sd 1.08)

\*  $an + 2cc = geh + wo + 2CO_2$  (Hoschek, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.64	1.0	840	230.49			896	10	** NOT USED **
0	0.57	1.0	865		237.01	20	885	10	cH = 240.71 (sd 0.89)
0	0.85	1.0	860	229.16	235.35	31	926	10	

\*  $2zo + CO_2 = 3an + cc + H_2O$  (Allen & Fawcett, 1982)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.07	5.0	590	38.09			652	16	** NOT USED **
0	0.08	5.0	610		39.85	22	632	14	cH = 40.86 (sd 0.34)
0	0.16	5.0	492	37.91			548	12	
0	0.19	5.0	505		39.39	27	532	12	
0	0.11	5.0	540	38.46			589	14	
0	0.12	5.0	560		39.93	19	579	14	

122)  $cc + q + and = an + CO_2$  (Chernosky & Berman, 1991)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.74	1.0	338	366	80.19	83.50	338	6	3 (81.85 <-> 83.58)
0	0.68	2.0	392	412	81.86	84.10	-15	377	6 cH = 80.19 (sd 0.35) 2
0	0.53	2.0		399		83.53	370	6	too low
0	0.82	2.0		409		82.91	384	6	uH = 0.62, d/s = 0.5, h = 0.04
0	0.17	2.0	364		82.27	-16	348	6	
0	0.21	2.0		379		83.57	352	6	

\*  $cc + q + and = an + CO_2$  (Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.27	2.0	390	410	84.26	86.69	-33	357	6 ** NOT USED **
0	0.69	2.0	440	460	87.15	89.37	-62	378	6 cH = 80.19 (sd 0.35)

\*  $cc + q + ky = an + CO_2$  (Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.17	6.0	490	510	85.80	88.31	-10	480	6 ** NOT USED **
0	0.75	6.0	565	585	89.06	91.20	-42	523	6 cH = 84.55 (sd 0.35)

## MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

123) **per + cor = sp** (Chamberlin et al., 1995)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.78	-	0.0	1200	-24.92	-23.06		2.74	0.05	1 (-24.85 <-> -23.80)
2.86	-	0.0	1200	-27.51	-22.46		2.74	0.05	cH = -23.48 (sd 0.31)
2.95	-	0.0	1250	-29.68	-23.73	-0.02	2.69	0.05	too high but OK
2.82	-	0.0	1300	-28.32	-23.08		2.65	0.05	uH = 0.36, d/s = 1.7, h = 0.17

124) **3en + 2cor = 2py** (Gasparik & Newton, 1984)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.35	-	16.0	850	52.11	52.72		16.49	0.74	2 (51.59 <-> 53.24)
									cH = 52.71 (sd 0.46)
									within bracket
									uH = 0.70, d/s = 0.4, h = 0.34

125) **2py + 2q = 3en + 2sill** (Perkins, 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.45	-	17.2	1600	-53.26	-51.21		16.55	0.60	3 (-54.25 <-> -52.20)
-0.63	-	18.0	16.9	-54.23	-52.24		16.67	0.59	cH = -52.35 (sd 0.47) 2
-0.82	-	19.1	18.5	-54.44	-53.08	-0.88	17.62	0.59	within bracket
									uH = 0.87, d/s = 0.1, h = 0.12

\* **2py + 2q = 3en + 2sill** (Hensen & Essene, 1971)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.45	-	15.3	14.4	-50.60	-49.33	1.25	16.55	0.60	** NOT USED **
-0.56	-	16.2	14.4	-52.01	-49.46	0.24	16.44	0.59	cH = -52.35 (sd 0.47)
-0.75	-	17.1	16.2	-52.02	-50.74	0.23	17.33	0.59	
-0.99	-	19.8	18.9	-53.49	-52.21		19.00	0.59	

126) **fo + py = sp + 2en** (Dankwerth & Newton, 1978; Gasparik & Newton, 1984)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.19	-	18.8	18.0	-25.10	-24.49		18.35	0.42	3 (-25.17 <-> -23.91)
-0.23	-	19.2	18.4	-24.92	-24.31		18.99	0.42	cH = -24.76 (sd 0.16)
-0.26	-	19.6	18.9	-24.89	-24.35		19.43	0.42	within bracket
-0.28	-	20.1	19.5	-24.87	-24.41		19.96	0.42	uH = 0.54, d/s = 0.2, h = 0.45
-0.30	-	20.6	19.7	-24.79	-24.10		20.56	0.42	
-0.35	-	22.0	21.2	-24.75	-24.15	0.01	22.01	0.43	
-0.49	-	29.9	29.0	-24.87	-24.22		29.74	0.44	

127) **en + sp = mgts + fo** (Gasparik & Newton, 1984)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.90	-	19.0	1020	29.25	29.63	14	1054	12	4 (29.24 <-> 30.48)
-1.52	-	10.2	1290	29.89	30.21		1290	14	cH = 29.89 (sd 0.12)
-1.45	-	19.9	1390	29.90	30.20		1390	16	within bracket
-1.39	-	11.8	1390	29.59	29.89		1410	16	uH = 0.37, d/s = -0.6, h = 0.86
-1.32	-	21.7	1490	29.47	29.75	10	1520	16	
-1.32	-	13.8	1490	30.06	30.35	-11	1479	16	
-1.27	-	25.7	1590	29.69	29.97		1604	18	
-1.27	-	21.8	1590	29.98	30.27	-7	1583	18	
-2.20	-	18.5	890	29.71	30.14		898	12	
-1.99	-	19.3	990	29.64	30.03		1003	12	
-1.27	-	29.5	1590	29.42	29.70	14	1624	18	

128) en + mgts = py (Perkins et al., 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
3.54	-	31.0	33.0	900	-6.53	-5.04	32.87	0.47	3 (-6.03 <-> -4.48)
2.81	-	29.0	31.0	1100	-6.17	-4.63	30.34	0.45	cH = -5.13 (sd 0.17)
3.47	-	39.0	41.0	1100	-6.21	-4.76	40.48	0.48	within bracket
2.42	-	21.0	23.0	1000	-5.60	-4.00	21.58	0.44	uH = 0.64, d/s = 0.2, h = 0.44
2.12	-	20.0	22.0	1100	-5.38	-3.76	20.31	0.43	
2.01	-	26.0	28.0	1400	-6.33	-4.73	27.49	0.44	
2.25	-	34.0	36.0	1500	-6.18	-4.64	35.35	0.45	
2.01	-	34.0	36.0	1600	-5.35	-3.80	34.28	0.45	
2.41	-	17.5	19.5	900	-6.08	-4.46	18.66	0.43	
2.25	-	18.3	20.3	1000	-5.99	-4.37	19.36	0.43	
1.76	-	28.5	30.5	1600	-5.90	-4.30	29.45	0.44	

129) 5en + 2sp = 5fo + crd (Herzberg, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.84	-	2.2	1.8	1150	28.00	30.26	2.02	0.22	3 (28.22 <-> 31.19)
0.90	-	2.0	1.6	1200	28.52	30.78	1.91	0.22	cH = 29.03 (sd 0.60)
1.02	-	1.7	1.3	1300	28.71	30.97	1.64	0.22	within bracket
									uH = 1.26, d/s = 0.6, h = 0.41

130) 5en + 2sp = crd + 5fo (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.55	-	3.3	2.8	905	29.07	31.15	0.01	0.22	3 (28.83 <-> 31.49)
0.67	-	3.2	2.7	1000	28.87	30.95	3.16	0.22	cH = 29.03 (sd 0.60) 2
0.78	-	2.9	2.4	1100	29.13	31.21	2.92	0.22	within bracket
									uH = 1.12, d/s = 0.8, h = 0.13

131) en + 3sill = crd + cor (Newton, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.12	-	10.5	10.0	825	9.32	10.65	0.08	0.17	2 (9.78 <-> 11.22)
0.14	-	10.5	10.0	875	10.35	11.68	0.47	0.17	cH = 9.10 (sd 0.37) 2
									too low but OK
									uH = 0.59, d/s = 0.2, h = 0.10

132) en + 2sill + q = crd (Newton, pers comm)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.17	-	7.4	6.8	950	9.65	12.33	0.08	0.16	1 (9.87 <-> 12.11)
									cH = 9.28 (sd 0.36)
									too low but OK
									uH = 0.68, d/s = 2.0, h = 0.08

133) clin = en + fo + sp + 4H2O (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.02	0	14.0	845	860	401.32	404.61	-5	840	4
									1 (401.37 <-> 404.56)
									cH = 400.19 (sd 0.43)
									too low
									uH = 1.19, d/s = 1.4, h = 0.06

134) ames = en + 2sp + 4H2O (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.88	0	14.0	845	860	394.00	397.29		849	6
									1 (394.04 <-> 397.25)
									cH = 394.92 (sd 0.65)
									within bracket
									uH = 1.20, d/s = 1.4, h = 0.13

135)  $afchl = en + 2fo + 4H2O$  (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
3.77	0	14.0	780	359.40	379.62	-1.87	6.80	0.12	5 (344.95 <-> 349.03)
6.82	0	14.0	800	343.70	348.69	-0.08	7.18	0.12	cH = 342.99 (sd 0.51) 2
7.47	0	14.0	840	344.40	349.58	-0.15	7.90	0.11	too low
									uH = 0.98, d/s = -5.5, h = 0.03

136)  $afchl = en + 2fo + 4H2O$  (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
7.81	0	10.0	800	340.51	345.07		7.78	0.12	5 (340.53 <-> 344.52)
7.50	0	12.0	800	339.98	344.98		7.45	0.12	cH = 342.99 (sd 0.51) 2
7.28	0	14.0	800	339.51	344.75		7.18	0.12	within bracket
6.23	0	16.0	800	337.59	361.51		6.97	0.12	uH = 0.92, d/s = -0.2, h = 0.04
4.91	0	18.0	800	345.13	374.35	-0.24	6.79	0.12	

137)  $2ames = afchl + 2cor + 2sp + 4H2O$  (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-6.33	0	14.0	780	438.14	442.09	-0.16	-6.71	0.25	1 (438.16 <-> 442.07)
-5.77	0	14.0	800	435.63	445.67		-6.08	0.24	cH = 443.49 (sd 1.07) 2
-5.05	0	14.0	820	436.55	442.71	-0.09	-5.48	0.24	too high but OK
									uH = 1.49, d/s = 1.3, h = 0.11

138)  $2ames = afchl + 2cor + 2sp + 4H2O$  (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-5.97	0	12.0	800	444.15	446.69	-0.07	-5.75	0.24	3 (443.00 <-> 446.51)
-5.66	0	14.0	800	435.63	443.73		-6.08	0.24	cH = 443.49 (sd 1.07) 2
-6.52	0	16.0	800	443.16	446.54		-6.37	0.24	within bracket
									uH = 1.49, d/s = -0.1, h = 0.17

139)  $4clin = 3afchl + 2cor + 2sp + 4H2O$  (Baker & Holland, 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-26.04	0	14.0	780	564.78	563.67	-0.45	-26.54	0.25	** NOT USED **
-25.39	0	14.0	800	568.86	563.80		-25.65	0.25	cH = 568.68 (sd 1.11)
-24.40	0	14.0	820	567.54	562.79	-0.13	-24.79	0.24	

\*  $clin = en + fo + sp + 4H2O$  (Fawcett & Yoder, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.03	0	3.0	725 755	399.88	408.23		726	4	** NOT USED **
0.02	0	5.0	770 790	403.00	408.15	-11	759	4	cH = 400.19 (sd 0.43)
0	0	10.0	815 840	401.10	406.89	-4	811	4	

140)  $clin = en + fo + sp + 4H2O$  (Jenkins, 1981; Jenkins & Chernosky, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.03	0	6.1	775 790	400.49	404.24	-1	774	4	3 (402.29 <-> 405.37)
0.02	0	8.0	810 820	404.01	406.41	-16	794	4	cH = 400.19 (sd 0.43) 2
0.02	0	12.0	840 850	403.12	405.37	-13	827	4	too low
0.02	0	14.0	850 860	402.42	404.61	-10	840	4	uH = 1.31, d/s = 0.1, h = 0.07

141)  $clin + 2cor = py + 2sp + 4H2O$  (Ackermann & Seifert, 1975)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.20	0	23.0	850 925	426.13	442.77		859	6	1 (426.60 <-> 430.64)
0.20	0	25.0	875		431.27		861	6	cH = 428.14 (sd 0.62) 2
0.20	0	26.0	825 875	420.17	431.12		861	6	within bracket
									uH = 1.12, d/s = 2.2, h = 0.00

142) 2mcar = sud + q (Vidal et al., 1992)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.30	-	7.6 6.9	350	36.78	37.72	-4.75	2.15	0.99	4 (42.86 <-> 45.45)
-0.30	-	7.7 6.5	400	43.35	44.96		7.10	1.02	cH = 44.15 (sd 0.66)
-0.30	-	6.3	500	59.90		-108	392	10	within bracket
-0.30	-	7.0	475		55.15		399	10	uH = 0.78, d/s = -14.3, h = 1.00

\* 2clin = py + 3fo + sp + 8H2O (Staudigel & Schreyer, 1977)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.33	0	20.4	890 900	833.46	837.53	-20	870	4	** NOT USED **
0.33	0	23.3	890 900	831.11	835.09	-15	875	4	cH = 825.14 (sd 0.87)
0.33	0	28.0	875 880	823.03	824.96		880	4	
0.33	0	32.6	870 880	820.33	824.08	3	883	6	

143) 3clin + 14q = 3ky + 5ta + 7H2O (Massonne et al., 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.65	0	11.0	600 630	573.94	583.18	7	637	10	5 (567.47 <-> 572.79)
-0.42	0	15.0	560 580	567.15	573.12	41	621	12	cH = 585.28 (sd 1.63) 2
-0.26	0	20.0	480	554.87			586	12	too high
									uH = 1.80, d/s = -0.2, h = 0.11

144) 2clin + 3en = 7fo + crd + 8H2O (Jenkins & Chernosky, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.20	0	0.5	595 612	813.71	826.75	3	615	2	3 (824.08 <-> 833.25)
0.23	0	1.0	634 660	817.21	834.86		652	2	cH = 829.41 (sd 1.01) 2
0.27	0	2.0	690 705	828.02	837.11		692	4	within bracket
0.29	0	3.0	720 734	828.24	836.23		722	4	uH = 3.51, d/s = -0.2, h = 0.03

145) 5clin + crd = 10en + 7sp + 20H2O (Jenkins & Chernosky, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.01	0	3.5	733	1967.41			736	4	3 (1947.85 <-> 1967.34)
0.01	0	3.0	740		1988.16		728	4	cH = 1971.92 (sd 2.30) 2
0.12	0	4.0	730	1953.19			744	4	too high but OK
0.12	0	4.7	750		1968.06	3	753	4	uH = 6.98, d/s = 0.0, h = 0.01
0.12	0	5.0	744	1956.16			756	4	

146) 5clin = 10fo + 3sp + crd + 20H2O (Chernosky, 1974; McPhail et al., 1990)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.36	0	0.5	605 640	1993.02	2059.15		625	2	3 (2024.68 <-> 2043.91)
0.42	0	1.0	644 670	2001.05	2044.56		661	2	cH = 2029.98 (sd 2.19) 2
0.42	0	2.0	690 704	2016.92	2037.81		699	2	within bracket
0.42	0	1.0	636 662	1987.71	2031.15		661	2	uH = 8.16, d/s = -1.0, h = 0.03
0.42	0	2.0	710 719	2046.76	2060.21	-11	699	2	
0.42	0	3.0	726 750	2031.92	2065.63	-1	725	4	

\* 6clin + 29q = 8ta + 3crd + 16H2O (Chernosky, 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.84	0	2.0	504 540	1396.27	1436.36	21	561	6	** NOT USED **
-0.93	0	3.0	536 552	1411.09	1428.12	30	582	6	cH = 1459.51 (sd 3.18)
-1.12	0	4.0	572 596	1432.05	1456.62	3	599	6	

147) 6clin + 29q = 8ta + 3crd + 16H2O (Massonne, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.90	0	2.0	547 557	1444.57	1455.69	3	560	6	3 (1443.93 <-> 1457.08)
-1.06	0	4.0	580 600	1439.80	1460.23		599	6	cH = 1459.51 (sd 3.18) 2
-1.28	0	6.0	616 626	1446.47	1456.18	3	629	6	too high but OK
									uH = 5.58, d/s = 0.8, h = 0.12

148) 2ta + 6sill + q = 3crd + 2H2O (Newton, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.47	0	8.5	7.2	670	235.17	246.99	7.36	0.15	3 (239.72 <-> 244.75)
0.47	0	9.0	8.5	700	237.38	241.87	-0.40	8.10	0.16 cH = 245.52 (sd 1.10) 2
0.47	0	9.9	9.4	750	240.48	244.92	-0.07	9.33	0.16 too high but OK
0.47	0	11.0	10.3	800	241.87	248.02	10.58	0.16	uH = 2.09, d/s = -0.0, h = 0.11

149) 2ta + 6ky + q = 3crd + 2H2O (Massonne & Schreyer, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.45	0	6.7	6.0	625	284.07	292.94	6.31	0.13	1 (284.82 <-> 292.19)
									cH = 288.94 (sd 1.13) 2
									within bracket
									uH = 2.21, d/s = 2.0, h = 0.02

150) 2clin + 8ky + 11q = 5crd + 8H2O (Seifert & Schreyer, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.28	0	4.0	550	600	864.54	901.90	560	4	3 (869.46 <-> 880.36)
0.28	0	5.0	550	600	841.97	878.75	590	4	cH = 871.76 (sd 1.94) 2
0.28	0	6.0	620	640	871.21	885.61	621	4	within bracket
0.28	0	7.0	650	660	871.31	878.41	651	4	uH = 4.63, d/s = 0.8, h = 0.05

151) 2clin + 8and + 11q = 5crd + 8H2O (Seifert & Schreyer, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.33	0	2.0	490	520	822.62	844.11	510	4	3 (832.98 <-> 841.62)
0.33	0	3.0	530	550	831.38	845.24	538	6	cH = 836.90 (sd 1.91) 2
0.33	0	4.0	560	570	833.93	840.68	564	6	within bracket
0.33	0	5.0	580	600	830.46	843.69	590	6	uH = 3.67, d/s = 0.9, h = 0.10
0.33	0	6.0	600	630	827.66	847.15	614	6	

152) 2clin + 19and = 5crd + 11cor + 8H2O (Seifert, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.45	0	2.0	520	570	851.73	888.18	540	4	3 (863.68 <-> 872.32)
0.42	0	3.0	560	570	863.66	870.70	564	6	cH = 866.61 (sd 1.93) 2
0.40	0	4.0	580	600	862.59	876.32	586	6	within bracket
0.37	0	5.0	600	620	862.55	875.99	606	6	uH = 3.67, d/s = 0.8, h = 0.14
0.33	0	6.0	620	640	863.40	876.62	625	6	
0.30	0	7.0	640	655	864.62	874.40	643	6	

153) 2clin + 19sill = 5crd + 11cor + 8H2O (Seifert, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.45	0	3.0	560	570	808.72	815.23	565	6	3 (803.59 <-> 812.04)
0.35	0	5.0	600	620	798.65	811.00	621	6	cH = 811.87 (sd 1.97) 2
0.33	0	6.0	640	650	806.72	812.76	649	6	within bracket
0.30	0	7.0	655	670	800.00	808.90	675	6	uH = 3.59, d/s = 0.0, h = 0.15

154) 2clin + 19ky = 5crd + 11cor + 8H2O (Seifert, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.33	0	5.0	610	620	953.78	962.21	-5	605	4 6 (949.69 <-> 962.12)
0.33	0	6.0	640	650	951.75	960.05	-3	637	4 cH = 949.40 (sd 2.10) 2
0.33	0	7.0	655	670	937.78	950.07		669	4 too low but OK
									uH = 5.27, d/s = -0.4, h = 0.07

\* 5clin + 20cor = 3crd + 19sp + 20H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.70	0	1.0	680	690	2215.77	2234.64	-51	629	4 ** NOT USED **
0.70	0	2.0	705	720	2187.41	2212.98	-40	665	4 cH = 2120.01 (sd 4.18)
0.70	0	4.0	740	750	2154.62	2170.24	-22	718	6
0.70	0	6.0	740	780	2088.41	2147.94		761	6

155)  $\text{clin} + 2\text{mag} = 3\text{fo} + \text{sp} + 2\text{CO}_2 + 4\text{H}_2\text{O}$  (Chernosky & Berman, 1986)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0.12	0.50	1.0	555	565	577.78	583.45		564	2	3 (577.35 <-> 583.95)
0.12	0.50	2.0	600		582.15			601	2	cH = 582.91 (sd 0.62) 2
0.12	0.50	3.0	625		580.83			629	2	within bracket
0.11	0.50	4.0	645	665	579.39	589.08		652	2	uH = 2.80, d/s = 0.2, h = 0.01

156)  $3\text{mctd} = \text{py} + 2\text{cor} + 3\text{H}_2\text{O}$  (Chopin & Schreyer, 1983)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	29.0	750	770	316.89	320.77		759	12	1 (317.02 <-> 319.80)
0	0	33.0	750	770	316.10	319.93		763	12	cH = 318.54 (sd 1.12)
										within bracket
										uH = 0.97, d/s = 1.6, h = 0.75

157)  $8\text{mctd} + 3\text{cor} + 7\text{ky} = 2\text{mst} + 4\text{H}_2\text{O}$  (Schreyer, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	23.0	680	720	470.52	483.89		709	22	1 (478.12 <-> 483.50)
0	0	32.0	680	720	477.73	491.53		687	20	cH = 480.26 (sd 3.40)
										within bracket
										uH = 1.77, d/s = 1.7, h = 0.61

158)  $8\text{clin} + 51\text{ky} + 31\text{cor} = 10\text{mst} + 12\text{H}_2\text{O}$  (Massonne, 1995)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0.41	0	25.0	710	730	1691.67	1709.80	-5	705	38	1 (1690.52 <-> 1710.96)
										cH = 1686.68 (sd 16.75) 2
										too low but OK
										uH = 8.47, d/s = 1.1, h = 0.52

159)  $25\text{ta} + 12\text{mst} = 67\text{ky} + 41\text{py} + 49\text{H}_2\text{O}$  (Chopin & Sobolev, 1995)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
4.96	0	17.0	765	795	5438.40	5527.60	-7	758	14	1 (5464.71 <-> 5521.27)
2.36	0	30.0	700	730	5458.39	5536.85	-15	685	18	cH = 5418.32 (sd 21.11) 2
										too low
										uH = 16.20, d/s = 2.1, h = 0.16

160)  $3\text{mcar} + \text{q} = \text{ta} + 3\text{ky} + 5\text{H}_2\text{O}$  (Chopin & Schreyer, 1983)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.08	0	19.0	540	560	407.86	413.31		546	10	3 (407.49 <-> 411.33)
-0.06	0	24.0	550	570	406.41	411.69		562	10	cH = 409.62 (sd 1.35)
-0.05	0	28.5	560	580	406.20	411.36		573	12	within bracket
										uH = 1.38, d/s = 1.3, h = 0.85

161)  $14\text{mcar} = \text{clin} + 13\text{ky} + 3\text{ta} + 21\text{H}_2\text{O}$  (Chopin & Schreyer, 1983)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.30	0	18.0	535	560	1712.86	1742.44		538	12	3 (1710.81 <-> 1727.88)
-0.24	0	24.0	560		1712.80			563	12	cH = 1716.49 (sd 6.30) 2
-0.21	0	28.5	565	590	1700.65	1728.51		579	12	within bracket
										uH = 6.11, d/s = 1.3, h = 0.12

162)  $5\text{mcar} = \text{clin} + 4\text{ky} + 3\text{q} + 6\text{H}_2\text{O}$  (Chopin & Schreyer, 1983)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.09	0	14.5		510		490.76		501	12	3 (489.39 <-> 495.01)
-0.04	0	16.5	515	550	486.97	499.64		517	14	cH = 487.61 (sd 2.30) 2
0	0	19.0	539		489.18		-4	535	14	too low but OK
-0.01	0	18.0		564		500.68		528	14	uH = 2.01, d/s = 0.4, h = 0.04



163) 2ta + 3ky + H2O = 3tats + 2q (Hoschek, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-11.47	0	10.5	650	24.93			707	36	3 (28.86 <-> 31.99)
-11.47	0	9.5	690		31.31		681	36	cH = 30.42 (sd 1.78)
-12.87	0	15.5	680	26.20			718	32	within bracket
-12.87	0	14.5	720		33.19		695	32	uH = 1.12, d/s = 0.3, h = 1.00
-14.63	0	20.5	705	30.59		-1	704	28	
-14.63	0	19.5	745		38.23		684	28	

164) 2py + 6sp + 4cor = 3spr4 (Akermand et al., 1975; Doroshev & Malinovskiy, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.32	-	21.6 20.7	950	21.14	23.54	-1.98	18.72	0.76	3 (23.25 <-> 26.73)
-0.42	-	23.4 19.8	1000	18.98	28.59	-0.11	19.69	0.76	cH = 28.88 (sd 1.03) 2
-0.52	-	23.4 20.7	1050	21.62	28.84	-0.01	20.69	0.76	too high
-0.71	-	25.7 22.1	1150	20.58	30.15		22.57	0.76	uH = 1.48, d/s = -0.8, h = 0.33
-0.82	-	25.8 24.8	1200	23.13	25.77	-1.17	23.63	0.77	
-0.94	-	27.5 25.6	1250	21.56	26.55	-0.88	24.72	0.77	
-1.16	-	27.9 26.1	1350	26.00	30.74		26.80	0.78	
-1.25	-	29.5 27.6	1400	24.36	29.33		27.77	0.78	

165) 6py = 7en + spr4 + 2sill (Hensen, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-2.45	-	16.5 15.5	1200	-115.67	-110.03		15.91	0.38	1 (-115.92 <-> -109.77)
-3.39	-	20.0 18.0	1400	-119.31	-108.11		18.75	0.38	cH = -112.32 (sd 1.06) 2
									within bracket
									uH = 2.50, d/s = 1.1, h = 0.03

166) 5spr4 = 2crd + 16sp (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.26	-	4.0 3.5	790	-67.50	-63.95	-0.28	3.22	0.29	5 (-65.00 <-> -61.78)
0.42	-	4.0 3.2	900	-66.45	-60.84		3.36	0.29	cH = -61.94 (sd 1.46) 2
0.53	-	3.7 3.5	955	-63.82	-62.43	-0.07	3.43	0.30	within bracket
0.93	-	3.4 3.2	1105	-60.58	-59.20	0.20	3.60	0.30	uH = 1.14, d/s = -1.5, h = 0.79

167) 2clin + 8cor + 2sp = 3spr4 + 8H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.12	0	2.0	680 700	892.53	906.09	-11	669	6	3 (887.29 <-> 895.12)
-0.12	0	3.0	700 730	891.19	910.46	-9	691	6	cH = 885.17 (sd 1.73) 3
-0.12	0	4.0	700 720	880.08	892.48		708	6	too low but OK
-0.12	0	5.0	730 760	889.09	907.13	-7	723	6	uH = 3.32, d/s = -0.9, h = 0.06
-0.12	0	6.0	730 740	880.94	886.82		737	6	
-0.12	0	7.0	740 760	879.56	891.09		750	6	

168) 16clin + 64cor = 2crd + 19spr4 + 64H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.20	0	2.0	680 690	7072.67	7127.02	-10	670	4	3 (7063.09 <-> 7124.20)
-0.20	0	4.0	710 730	7002.34	7101.78		713	6	cH = 7019.38 (sd 13.47) 3
-0.20	0	5.0	740 750	7063.22	7111.52	-9	731	6	too low
-0.20	0	6.0	760 775	7081.05	7151.77	-13	747	6	uH = 25.94, d/s = 0.4, h = 0.05

169) 16clin + 6crd = 32en + 7spr4 + 64H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.69	0	4.0	760 770	6531.20	6572.98	-32	728	4	2 (6484.01 <-> 6533.79)
-1.69	0	7.0	755 765	6448.26	6486.60	-13	742	4	cH = 6396.87 (sd 7.57) 3
									too low
									uH = 21.13, d/s = -1.1, h = 0.02

\* 2clin + 8cor + 2sp = 3spr4 + 8H2O (Akermand et al., 1975)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.09	0	10.0	700 800	838.02	892.93		786	6	** NOT USED **
0.09	0	13.0	750 800	851.42	877.85	14	814	6	cH = 885.17 (sd 1.73)
0.09	0	15.0	775 840	856.35	889.86		831	6	
0.09	0	19.0	835 870	872.01	889.31		862	8	
0.09	0	23.0	870 900	875.94	890.25		889	8	
0.09	0	25.0	900	884.07			902	8	

170) py + 4sp + 4cor = 2spr7 (Akermand et al., 1975; Doroshev & Malinovskiy, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.21	-	21.6 20.7	950	46.74	48.49	-1.89	18.81	0.81	3 (48.42 <-> 50.80)
-0.17	-	23.4 19.8	1000	45.29	52.28		19.84	0.81	cH = 52.20 (sd 0.80) 2
-0.12	-	23.4 20.7	1050	47.22	52.47		20.84	0.81	too high but OK
-0.06	-	25.7 22.1	1150	46.71	53.67		22.85	0.82	uH = 1.01, d/s = -0.9, h = 0.38
-0.04	-	25.8 24.8	1200	48.49	50.41	-0.92	23.88	0.82	
-0.02	-	27.5 25.6	1250	47.16	50.79	-0.73	24.87	0.82	
0	-	27.9 26.1	1350	50.31	53.76		26.91	0.83	
0	-	29.5 27.6	1400	49.29	52.91		27.97	0.83	

171) 13py = 16en + 2spr7 + 4sill (Hensen, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-4.84	-	16.5 15.5	1200	-233.52	-221.22		15.96	0.38	1 (-234.17 <-> -220.57)
-6.65	-	20.0 18.0	1400	-241.46	-217.03		18.80	0.38	cH = -226.83 (sd 2.30) 2
									within bracket
									uH = 5.58, d/s = 1.1, h = 0.03

172) 2spr7 + en = crd + 7sp (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.29	-	4.0 3.5	790	-42.94	-41.22		3.59	0.26	3 (-42.80 <-> -41.53)
0.32	-	4.0 3.2	900	-43.66	-40.95		3.37	0.26	cH = -41.53 (sd 0.64) 2
0.33	-	3.7 3.5	955	-42.88	-42.21	-0.20	3.30	0.27	within bracket
0.37	-	3.4 3.2	1105	-42.22	-41.55	-0.00	3.20	0.27	uH = 0.54, d/s = 0.0, h = 0.72

173) clin + 6cor + 2sp = 2spr7 + 4H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.03	0	2.0	680 700	484.77	492.27	-12	668	6	3 (481.77 <-> 486.15)
-0.03	0	3.0	700 730	484.14	494.85	-11	689	6	cH = 480.34 (sd 1.14) 3
-0.03	0	4.0	700 720	477.92	484.83		707	6	too low but OK
-0.03	0	5.0	730 760	482.82	492.91	-7	723	6	uH = 1.86, d/s = -0.9, h = 0.08
-0.03	0	6.0	730 740	478.08	481.38		737	6	
-0.03	0	7.0	740 760	477.09	483.56		750	8	

174) 29clin + 154cor = 6crd + 38spr7 + 116H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.45	0	2.0	680 690	13475.57	13581.09	-10	670	6	3 (13430.89 <-> 13556.01)
0.45	0	4.0	710 730	13318.93	13513.20		715	6	cH = 13366.51 (sd 29.04) 3
0.45	0	5.0	740 750	13425.38	13519.96	-6	734	6	too low
0.45	0	6.0	760 775	13446.92	13585.63	-9	751	6	uH = 53.09, d/s = 0.4, h = 0.07

175) 5clin + 20spr7 = 9crd + 77sp + 20H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.58	0	2.0	700 710	1570.74	1584.72	-10	690	10	4 (1543.93 <-> 1573.28)
2.58	0	3.0	730		1533.18	18	748	10	cH = 1556.58 (sd 6.88) 3
2.58	0	4.0	760 780	1502.33	1528.06	22	802	10	within bracket
									uH = 8.82, d/s = -2.4, h = 0.10

176) 5clin + 2crd = 1len + 2spr7 + 20H2O (Seifert, 1974)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.86	0	4.0	760	770	2056.18	2069.39	-32	728	4	2 (2042.13 <-> 2057.95)
-0.86	0	7.0	755	765	2031.77	2043.90	-15	740	4	cH = 2013.46 (sd 2.38) 3
										too low
										uH = 6.71, d/s = -0.9, h = 0.02

\* clin + 6cor + 2sp = 2spr7 + 4H2O (Akermand et al., 1975)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.05	0	10.0	700	800	453.95	485.02		785	8	** NOT USED **
-0.12	0	13.0	750	800	461.12	476.15	14	814	8	cH = 480.34 (sd 1.14)
-0.16	0	15.0	775	840	463.64	482.77		832	8	
-0.28	0	19.0	835	870	472.30	482.26		863	8	
-0.36	0	23.0	870	900	473.88	482.16		893	8	
-0.41	0	25.0	900		478.40			907	8	

177) 2ged + 6ky + 7q = 5crd + 2H2O (Schreyer & Seifert, 1969)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
3.93	0	11.0 10.0	850		264.90	280.85		10.50	1.19	1 (266.40 <-> 279.35)
										cH = 272.88 (sd 14.75) 2
										within bracket
										uH = 3.63, d/s = 2.2, h = 1.00

## CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>

178)  $ts + 2di + 2q = tr + 2an$  (Jenkins, 1994)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.76	-	2.0	607	-23.42	-6.41	miss	4.99	0.62	1 (-9.49 <-> -6.76)
5.47	-	2.0	698	-22.01	-6.06		4.88	0.56	cH = -9.28 (sd 2.27) 2
4.85	-	2.0	797	-16.57	-3.28		4.77	0.51	within bracket
3.93	-	4.5	674	-12.54	-3.54		4.09	0.58	uH = 0.45, d/s = 3.8, h = 0.23
3.81	-	4.5	776	-11.58	-2.58		4.06	0.52	
2.93	-	7.0	650	-9.84	-3.91		3.24	0.59	
3.10	-	7.0	750	-14.11	-0.72		3.32	0.53	

179)  $ts + 2fo = tr + 2sp$  (Jenkins, 1994)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.56	-	5.9	789	-29.54	-25.39	miss	1.40	0.50	1 (-26.41 <-> -25.49)
1.41	-	6.1	800	-28.31	-24.35		1.38	0.49	cH = -26.07 (sd 2.19) 2
1.25	-	8.0	827	-26.50	-22.67		1.41	0.48	within bracket
									uH = 0.27, d/s = 2.0, h = 0.67

180)  $5ts + 7q = 3tr + 7ky + 2zo + H_2O$  (Hoschek, 1995)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
8.60	0	10.0	700	-68.46	-29.17		7.63	2.71	1 (-67.49 <-> -39.95)
13.96	0	15.0	720	-75.41	-38.98		12.00	2.66	cH = -41.00 (sd 10.98) 2
17.05	0	20.0	740	-80.98	-16.96		16.10	2.61	within bracket
									uH = 2.41, d/s = 6.1, h = 0.13

181)  $clin + 2dol = 3fo + 2cc + sp + 4H_2O + 2CO_2$  (Chernosky & Berman, 1986)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.04	0.43	1.0	565 585	585.76	597.14		579	4	1 (586.68 <-> 596.22)
									cH = 593.77 (sd 0.95) 2
									within bracket
									uH = 2.92, d/s = 2.0, h = 0.01

182)  $3clin + 2cc = 2di + 5fo + 3sp + 2CO_2 + 12H_2O$  (Chernosky & Berman, 1986)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.09	0.20	1.0	588 608	1326.59	1350.63		608	2	1 (1328.55 <-> 1348.67)
									cH = 1350.63 (sd 1.56) 2
									too high but OK
									uH = 6.12, d/s = 2.0, h = 0.00

183)  $25pump = 29cz + 14gr + 5clin + 6q + 53H_2O$  (Schiffman & Liou, 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.26	0	5.0	360 380	3809.74	3859.71	-15	345	6	4 (3746.78 <-> 3790.19)
-0.26	0	6.0	359 365	3760.85	3776.12		362	6	cH = 3768.50 (sd 11.24)
-0.26	0	8.0	377 395	3720.19	3759.27	5	400	8	within bracket
									uH = 13.04, d/s = -1.9, h = 1.00

184)  $2vsv + 6q = 11gr + 4di + wo + 9H_2O$  (Hochella et al., 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	375 390	462.97	464.92		377	4	2 (462.10 <-> 464.51)
0	0	2.0	400 415	460.79	463.64		413	6	cH = 463.31 (sd 0.82)
									within bracket
									uH = 0.87, d/s = 0.4, h = 1.00

## Na<sub>2</sub>O–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>

185)  $jd + q = abh$  (Holland, 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	16.5 16.0	600	13.21	14.04		16.11	0.33	3 (13.18 <-> 15.01)
0	-	22.0 21.0	800	13.24	14.87		21.61	0.34	cH = 13.87 (sd 0.28)
0	-	25.0 23.5	900	12.84	15.26		24.36	0.34	within bracket
0	-	27.5 26.0	1000	13.22	15.61		27.09	0.34	uH = 0.77, d/s = 0.3, h = 0.40
0	-	30.0 29.0	1100	13.58	15.15		29.82	0.35	
0	-	33.0 31.0	1200	13.13	16.24		32.52	0.35	

186)  $jd + q = ab$  (Newton & Smith, 1967; Holland, 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	15.2 13.5	500	2.67	5.42		14.31	0.35	3 (3.52 <-> 5.32)
0	-	15.7 14.9	550	3.77	5.07		15.49	0.35	cH = 4.11 (sd 0.28) 2
0	-	16.9 16.2	600	3.77	4.90		16.69	0.35	within bracket
0	-	22.0 21.0	800	3.59	5.20		21.68	0.36	uH = 0.76, d/s = 0.7, h = 0.14
0	-	25.0 23.5	900	3.08	5.50		24.36	0.36	
0	-	27.5 26.0	1000	3.46	5.85		27.09	0.37	
0	-	30.0 29.0	1100	3.81	5.39		29.81	0.37	
0	-	33.0 31.0	1200	3.36	6.47		32.51	0.37	

187)  $jd + ky = abh + cor$  (Essene et al., 1972)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	19.5 18.5	800	19.18	21.24		18.65	0.28	2 (19.77 <-> 22.11)
0	-	29.3 28.3	1200	20.64	22.61		29.15	0.29	cH = 20.93 (sd 0.28) 2
									within bracket
									uH = 1.00, d/s = 0.3, h = 0.02

188)  $2jd = ne + abh$  (Gasparik, 1985; Robertson et al., 1957; Boettcher & Wyllie, 1968)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	11.0 10.0	600	32.87	36.30		10.14	0.54	3 (34.04 <-> 37.32)
0	-	15.0 14.0	800	35.16	38.55		14.81	0.55	cH = 35.81 (sd 0.92)
0	-	18.3 15.4	825	26.02	35.77	-0.01	15.39	0.55	within bracket
0	-	19.5 18.0	950	31.72	36.75		18.28	0.55	uH = 1.37, d/s = 0.0, h = 0.97
0	-	21.0	1050	34.40			1069	24	
0	-	20.0	1100		41.55		1025	24	
0	-	24.0 23.0	1200	35.76	39.08		23.99	0.56	

189)  $pa = jd + ky + H_2O$  (Holland, 1979)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	24.0 26.0	550	81.73	83.83		25.74	0.56	3 (83.07 <-> 84.33)
0	0	24.0 25.5	600	82.65	84.23		24.86	0.56	cH = 83.56 (sd 0.29)
0	0	24.0 25.0	650	83.54	84.59		24.02	0.56	within bracket
0	0	23.0 24.5	700	83.35	84.92		23.21	0.56	uH = 0.53, d/s = 0.3, h = 0.51

190)  $pa = abh + cor + H_2O$  (Chatterjee, 1970)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	530 550	104.93	106.84	-5	525	4	3 (104.95 <-> 106.11)
0	0	2.0	555 575	104.73	106.49	-3	552	4	cH = 104.49 (sd 0.20)
0	0	3.0	580 600	104.88	106.56	-5	575	4	too low
0	0	5.0	625 640	105.16	106.37	-8	617	6	uH = 0.43, d/s = 0.5, h = 0.36
0	0	6.0	620 650	103.25	105.61		636	6	
0	0	7.0	650 670	104.17	105.72		654	6	

191)  $pa + q = abh + and + H2O$  (Chatterjee, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	470 490	98.90	100.74	11	501	4	3 (100.25 <-> 101.31)
0	0	2.0	510 530	100.02	101.76		530	4	cH = 101.79 (sd 0.20)
0	0	3.0	540 560	100.41	102.08		557	4	too high
0	0	4.0	560 580	100.07	101.70	1	581	4	uH = 0.45, d/s = 0.1, h = 0.36
0	0	5.0	590 600	100.61	101.41	5	605	6	

192)  $pa + q = abh + ky + H2O$  (Chatterjee, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	5.0	570 625	94.95	98.82		605	6	1 (96.53 <-> 97.69)
0	0	6.0	600 630	96.02	98.10		620	6	cH = 97.43 (sd 0.20)
0	0	7.0	620 640	96.43	97.79		635	6	within bracket
									uH = 0.36, d/s = 1.9, h = 0.15

193)  $jd + H2O = anl$  (Manghnani, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	11.0 6.4	350	-48.73	-40.16		6.46	0.38	1 (-41.38 <-> -40.28)
0	0	9.0 7.5	450	-42.29	-39.60		7.87	0.38	cH = -40.26 (sd 0.34) 2
0	0	9.5 8.0	500	-41.95	-39.30		8.55	0.39	too high but OK
0	0	10.0 8.0	550	-41.50	-38.02		9.30	0.39	uH = 0.32, d/s = 2.1, h = 0.06
0	0	11.0 9.0	575	-42.54	-39.05		9.70	0.39	

194)  $anl + q = abh + H2O$  (Thompson, 1971; Liou, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	180 200	53.81	54.39		191	4	3 (53.93 <-> 54.30)
0	0	4.0	160 180	53.50	53.99	4	184	4	cH = 54.13 (sd 0.21) 2
0	0	3.0	190 205	54.15	54.57	-1	189	4	within bracket
0	0	4.0	175 195	53.86	54.39		185	4	uH = 0.13, d/s = -0.6, h = 0.98
0	0	5.0	175 190	54.02	54.40		179	4	

## K<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

195) **mic = san** (Carpenter et al., 1994)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	445	460	10.05	10.26		452	16	1 (10.06 <-> 10.25) cH = 10.16 (sd 0.11) within bracket uH = 0.07, d/s = 1.5, h = 1.00

196) **mu = san + cor + H<sub>2</sub>O** (Chatterjee & Johannes, 1974)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	600	630	102.69	105.23	-5	595	4	3 (102.42 <-> 103.32)
0	0	2.0	640	660	102.83	104.34	-8	632	4	cH = 102.22 (sd 0.17)
0	0	4.0	690	710	102.21	103.59		690	6	too low but OK
0	0	6.0	740	750	102.18	102.83		741	6	uH = 0.38, d/s = 0.0, h = 0.34
0	0	8.0	780	800	101.74	102.98		788	6	

197) **mu + q = san + and + H<sub>2</sub>O** (Chatterjee & Johannes, 1974)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	520	560	97.73	101.54		539	4	3 (98.47 <-> 99.36)
0	0	1.0	550	570	97.96	99.61		569	4	cH = 99.52 (sd 0.17)
0	0	2.0	590	605	98.17	99.28	3	608	4	too high but OK
0	0	3.0	620	640	97.96	99.37	2	642	4	uH = 0.38, d/s = 0.9, h = 0.42
0	0	4.0	660	670	98.59	99.27	4	674	6	
0	0	5.0	690	705	98.60	99.57		704	6	

198) **mu + q = san + sill + H<sub>2</sub>O** (Chatterjee & Johannes, 1974)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	540	580	102.00	105.90		544	4	3 (101.87 <-> 102.91)
0	0	2.0	595	630	101.33	104.01		609	4	cH = 102.40 (sd 0.17)
0	0	3.0	630	660	101.74	103.92		639	4	within bracket
0	0	5.0	680	705	101.55	103.25		692	6	uH = 0.44, d/s = 0.7, h = 0.24
0	0	6.0	710	720	101.91	102.57		717	6	

## K<sub>2</sub>O–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>

199) **kals + san = 2lc** (Scarfe et al., 1965; Lindsley 1966)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	-	4.0	600	628	27.75	28.87		620	14	3 (28.31 <-> 28.95)
0	-	6.0	675	700	28.43	29.43		678	14	cH = 28.54 (sd 0.27)
0	-	8.0	725	750	28.08	29.08		737	14	within bracket
0	-	25.0 22.0	1200		26.14	29.89		22.84	0.77	uH = 0.23, d/s = 0.9, h = 0.94

200) **san + fo = lc + en** (Luth, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	-	1.0	975	1005	16.84	17.53		1001	22	1 (16.91 <-> 17.46)
										cH = 17.45 (sd 0.25)
										within bracket
										uH = 0.12, d/s = 3.0, h = 0.64

201) **2phl + 3en = 2san + 6fo + 2H<sub>2</sub>O** (Luth, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.4	850	900	260.69	270.26		873	14	1 (261.86 <-> 268.37)
0	0	0.7	905	950	261.11	269.13		927	16	cH = 265.12 (sd 1.38)
										within bracket
										uH = 0.97, d/s = 4.2, h = 0.23

202) **2phl + san = 3lc + 3fo + 2H<sub>2</sub>O** (Luth, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.4	900	950	315.99	328.96		906	10	1 (316.28 <-> 320.30)
0	0	0.7	940	960	315.64	320.58		947	12	cH = 317.47 (sd 1.43)
										within bracket
										uH = 1.33, d/s = 1.7, h = 0.41

\* **2phl = kals + lc + 3fo + 2H<sub>2</sub>O** (Luth, 1967)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.4	1000	1020	289.85	294.02	-4	996	14	** NOT USED **
0	0	0.7	1050	1075	288.74	293.68		1051	14	cH = 288.93 (sd 1.44)
0	0	1.0	1150	1175	300.60	305.36	-61	1089	16	

203) **kals + 2en = san + 2fo** (Wendlandt & Eggler, 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	-	27.0 25.0	1170		-8.13	-6.32		25.05	1.15	1 (-7.99 <-> -6.46)
										cH = -6.36 (sd 0.52)
										too high but OK
										uH = 0.47, d/s = 1.9, h = 0.36

\* **5mu + 3clin = 5phl + 8ky + q + 12H<sub>2</sub>O** (Bird & Fawcett, 1973)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-1.00	0	7.2	632	640	1062.65	1067.95	-11	621	12	** NOT USED **
-1.00	0	8.3	634	646	1060.44	1068.21	-8	626	12	cH = 1055.37 (sd 3.74)

\* **5mu + 3clin = 5phl + 8ky + q + 12H<sub>2</sub>O** (Massonne, unpub)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-1.68	0	4.0	540	570	1018.19	1040.11	21	591	10	** NOT USED **
-1.68	0	6.0	570	590	1030.12	1043.94	17	607	10	cH = 1055.37 (sd 3.74)



\* 6mu + 2phl + 15q = 3crd + 8san + 8H2O (Seifert, 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.46	0	1.0	520 530	846.34	853.58	12	542	6	** NOT USED **
1.46	0	2.0	580 600	860.26	873.63		583	6	cH = 862.22 (sd 2.10)
1.46	0	3.0	630 640	868.31	874.64	-10	620	6	
1.46	0	4.0	660 670	864.52	870.62	-4	656	6	
1.46	0	5.0	685 700	858.63	867.51		691	6	

\* mu + clin + 2q = crd + phl + 4H2O (Seifert, 1970)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.29	0	1.0	485 505	378.96	385.75		504	4	** NOT USED **
-0.29	0	2.0	515 535	380.47	386.81		531	6	cH = 385.43 (sd 0.85)
-0.29	0	5.0	595 625	385.50	394.13		595	6	
-0.29	0	6.0	625 645	388.63	394.25	-11	614	6	
-0.29	0	7.0	650 660	390.45	393.20	-18	632	6	

204) 6cel + 6ky + 2H2O = 2ta + 6mu + 4coe (Massonne & Schreyer, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-2.11	0	41.0 39.0	750	-224.93	-215.52	-0.89	38.11	1.87	5 (-223.36 <-> -213.80)
-2.54	0	41.0 39.0	670	-227.53	-218.02	-1.40	37.60	1.84	cH = -211.31 (sd 4.43) 3
0.42	0	36.0 34.0	770	-221.73	-212.14	-0.17	33.83	1.84	too high but OK
-1.25	0	36.0 34.0	666	-213.94	-204.22		35.46	1.82	uH = 3.67, d/s = -1.8, h = 0.58
1.22	0	36.0 34.0	587	-236.77	-226.94	-3.15	30.85	1.77	
2.41	0	31.0 29.0	754	-215.41	-205.61		30.16	1.81	
4.00	0	31.0 29.0	685	-230.15	-220.25	-1.79	27.21	1.77	
1.63	0	31.0 29.0	601	-214.40	-204.39		30.38	1.77	

205) 6cel + 6ky + 2H2O = 2ta + 6mu + 4q (Massonne & Schreyer, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
3.11	0	26.0 24.0	742	-216.30	-204.67	2.86	28.86	1.58	4 (-226.73 <-> -218.36)
5.46	0	26.0 24.0	656	-236.61	-224.87		25.35	1.54	cH = -232.78 (sd 4.43) 3
3.49	0	26.0 24.0	573	-223.30	-211.45	1.61	27.61	1.54	too low but OK
8.66	0	21.0 19.0	728	-233.63	-221.81		20.86	1.54	uH = 2.52, d/s = -3.9, h = 0.42
6.63	0	21.0 19.0	647	-216.10	-204.16	2.81	23.81	1.53	
14.52	0	16.0 14.0	663	-247.76	-235.74	-0.49	13.51	1.52	

\* 3cel = phl + 2san + 3q + 2H2O (Massonne & Schreyer, 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.94	0	21.0 19.0	645	150.54	159.65	-1.80	17.20	1.05	** NOT USED **
3.60	0	16.0 14.0	649	161.59	171.13		14.66	1.02	cH = 167.96 (sd 2.38)
4.92	0	11.6 9.6	590	164.03	174.01		10.81	0.98	
5.73	0	11.6 9.6	590	158.25	168.23		9.65	0.96	
5.29	0	11.6 9.6	689	175.57	185.81	1.53	13.13	1.00	
8.28	0	8.0 6.0	650	165.65	176.69		7.57	0.91	
10.83	0	6.0 4.0	700	162.46	174.87		5.09	0.81	

\* 3cel = phl + 2san + 3q + 2H2O (Velde, 1965; Massonne & Schreyer, 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
7.67	0	2.0	375 390	165.66	167.64	3	393	28	** NOT USED **
5.68	0	4.5	440 480	172.40	178.79	-28	412	26	cH = 167.96 (sd 2.38)

206) 3mu + 2phl = 3east + 2san + 3q + 2H2O (Massonne & Schreyer, 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-2.10	0	6.0 4.0	700	192.91	203.77		4.97	4.04	1 (193.78 <-> 202.90)
									cH = 198.34 (sd 10.40) 2
									within bracket
									uH = 1.16, d/s = 4.7, h = 1.00

\*  $ta + \mu = phl + ky + 3q + H_2O$  (Massonne & Schreyer, 1989)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0.06	0	10.0	595	623	91.18	92.95	17	640	24	** NOT USED **
0.28	0	15.0	662	675	91.18	91.92	37	712	26	cH = 94.02 (sd 0.72)
0.49	0	20.0	723	732	90.69	91.16	55	787	30	
0.70	0	25.0	771	790	89.25	90.16	81	871	32	

207)  $3clin + 3phl + 23q = 3\mu + 8ta + 4H_2O$  (Massonne & Schreyer, 1989)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-1.63	0	9.6	562		297.89			601	46	2 (304.51 <-> 309.22)
-1.63	0	14.0		544		308.49		505	44	cH = 303.23 (sd 2.91) 3
-0.91	0	10.6	639		305.24		-17	622	50	too low but OK
-0.91	0	13.0		619		309.72		566	48	uH = 1.69, d/s = 1.0, h = 0.13

208)  $2phl + 6q = 3en + 2san + 2H_2O$  (Bohlen et al., 1983)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.66	5.0	775	805	213.31	217.58	17	822	20	1 (213.77 <-> 217.12)
										cH = 219.95 (sd 1.37) 2
										too high
										uH = 0.74, d/s = 2.9, h = 0.13

209)  $2phl + 6q = 3en + 2san + 2H_2O$  (Peterson & Newton, 1990)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.73	2.5	745	765	218.51	221.69		754	18	1 (218.76 <-> 221.43)
										cH = 219.95 (sd 1.37) 2
										within bracket
										uH = 0.82, d/s = 1.9, h = 0.20

\*  $2phl + 6q = 3en + 2san + 2H_2O$  (Wood, 1976)

ln_K	x(CO2)	P(kbar)		T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	0.3	0.3	750	222.88	225.11	0.08	0.43	0.08	** NOT USED **
0	0	0.5	0.4	790	225.83	228.19	0.25	0.72	0.15	cH = 219.95 (sd 1.37)

$$\text{Na}_2\text{O}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2 \quad \& \quad \text{K}_2\text{O}-\text{CaO}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2$$

210)  $2jd + ta = ql$  (Carman & Gilbert, 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	37.0	35.0	800	-17.54	-16.09		35.82 2.18	1 (-17.52 <-> -16.12) cH = -16.69 (sd 0.79) within bracket uH = 0.52, d/s = 1.4, h = 0.98

211)  $2\text{naph} + 3\text{en} = 2\text{abh} + 6\text{fo} + 2\text{H}_2\text{O}$  (Carman & Gilbert, 1985)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.8	820	852	251.59	257.45	-5	815	14	2 (249.33 <-> 251.92)
0	0	1.6	850	870	246.36	249.67	6	876	16	cH = 250.63 (sd 1.37)
										within bracket
										uH = 0.93, d/s = -1.0, h = 1.00

212)  $5\text{phl} + 6\text{cc} + 24\text{q} = 3\text{tr} + 5\text{san} + 6\text{CO}_2 + 2\text{H}_2\text{O}$  (Hewitt, 1975)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.72	6.0	610	600.39			619	14	2 (602.89 <-> 611.41)
0	0.68	6.0	630		611.30		618	14	cH = 605.21 (sd 3.83) 2
0	0.58	6.0	610	603.00			614	14	within bracket
0	0.55	6.0	625		611.84		612	14	uH = 3.05, d/s = 1.4, h = 0.16

\*  $3\text{dol} + \text{san} + \text{H}_2\text{O} = \text{phl} + 3\text{cc} + 3\text{CO}_2$  (Puhan & Johannes, 1974; Puhan, 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.12	0.83	2.0	490	161.62		-18	472	14	** NOT USED **
-0.12	0.75	2.0	490		165.45		455	12	ch = 157.81 (sd 1.39)
-0.12	0.60	2.0	460	164.23		-28	432	12	
-0.12	0.47	2.0	470		170.46		417	12	
-0.19	0.80	4.0	550	158.90		-6	544	14	
-0.19	0.86	4.0	580		160.95		563	14	
-0.19	0.64	6.0	575	157.92		-1	574	14	
-0.22	0.59	6.0	575		159.96		564	14	

213)  $\mu + cc + 2q = san + an + CO_2 + H_2O$  (Hewitt, 1973)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.50	2.0	450	500	179.80	189.60		450	4	3 (181.18 <-> 183.61)
0	0.50	4.0	525	540	182.06	184.82	-13	512	4	cH = 179.72 (sd 0.39) 2
0	0.50	5.0	550	560	181.38	183.18	-9	541	4	too low
0	0.50	6.0	575	585	180.99	182.76	-7	568	4	uH = 1.03, d/s = 0.3, h = 0.08
0	0.50	7.0	605	615	181.69	183.42	-11	594	4	

\*  $2z_o + \mu + 2\alpha = 4\alpha_n + \alpha_n + 2H_2O$  (Johannes, 1980)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	4.0	470	490	213.02	217.83	11	501	4	** NOT USED **
0	0	4.8	510	520	215.22	217.60	12	532	4	cH = 220.57 (sd 0.43)
0	0	5.5	530	555	213.57	219.48	5	560	4	
0	0	6.0	555	570	214.93	218.46	9	579	4	
0	0	7.0	595	610	215.29	218.78	8	618	4	
0	0	8.8 8.0	660		214.33	221.38		8.09 0.10		

Na<sub>2</sub>O–CaO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>    &    Na<sub>2</sub>O–CaO–MgO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>

\*    4law + ab = 2zo + pa + 2q + 6H<sub>2</sub>O    (Heinrich & Althaus, 1980)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	7.0	360	400	400.86	411.85	-18	342	4	** NOT USED **
0	0	9.5	405	445	401.08	413.48	-22	383	4	cH = 395.25 (sd 0.95)
0	0	12.0	435	465	398.94	408.05	-12	423	6	

\*    4law + jd = 2zo + pa + q + 6H<sub>2</sub>O    (Heinrich & Althaus, 1980)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	12.0	435	465	404.34	414.59	-15	420	6	** NOT USED **
0	0	15.0	460	480	395.37	401.98		472	6	cH = 399.36 (sd 0.97)

214)    2parg + 5en = 2di + 8fo + 2an + 2abh + 2H<sub>2</sub>O    (Lykins & Jenkins, 1992)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-2.09	0	0.5	760	790	303.89	310.98		787	14	3 (308.21 <-> 312.43)
-2.09	0	1.0	828	860	307.02	313.91		843	16	cH = 310.32 (sd 1.66)
-2.09	0	1.5	880	900	309.61	313.66		884	16	within bracket
										uH = 1.66, d/s = 0.4, h = 1.00

## FeO-SiO<sub>2</sub>

215)  $fs = fa + q$  (Bohlen et al., 1980)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	10.7 10.3	700	-0.46	-0.35		10.32	0.28	3 (-0.44 <-> -0.27)
0	-	11.2 10.8	750	-0.44	-0.32		10.92	0.29	cH = -0.35 (sd 0.03)
0	-	11.7 11.3	800	-0.41	-0.29		11.52	0.30	within bracket
0	-	12.2 11.8	850	-0.37	-0.25		12.14	0.30	uH = 0.07, d/s = 0.2, h = 0.99
0	-	12.9 12.4	900	-0.39	-0.23		12.79	0.31	
0	-	13.5 13.1	950	-0.37	-0.25		13.44	0.32	
0	-	14.3 13.9	1000	-0.43	-0.30		14.06	0.33	
0	-	15.0 14.6	1050	-0.46	-0.34		14.65	0.34	

216)  $4mt + O_2 = 6hem$  (Myers & Eugster, 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
10.82	-	0.0	1053 1043	-490.23	-483.67	5	1058	6	3 (-490.87 <-> -486.05)
9.59	-	0.0	1083 1073	-487.71	-481.21	12	1095	6	cH = -492.19 (sd 1.19) 2
8.77	-	0.0	1113 1103	-489.21	-482.71	8	1121	6	too low but OK
8.06	-	0.0	1142 1132	-491.22	-484.73	3	1145	6	uH = 1.72, d/s = -0.5, h = 0.32
7.21	-	0.0	1172 1162	-491.69	-485.21	1	1173	6	
6.48	-	0.0	1201 1191	-492.68	-486.22		1200	8	
5.74	-	0.0	1228 1218	-492.72	-486.25		1226	8	
5.08	-	0.0	1262 1252	-495.64	-489.14		1251	8	
4.79	-	0.0	1274 1264	-495.81	-489.30		1263	8	

217)  $4mt + O_2 = 6hem$  (Chou, 1978)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
36.15	-	2.0	605 595	-505.21	-495.03	-11	584	4	3 (-498.42 <-> -491.61)
31.64	-	2.0	655 645	-500.91	-491.01		640	4	cH = -492.19 (sd 1.19)
27.38	-	2.0	705 695	-494.12	-488.59		701	4	within bracket
24.96	-	2.0	755 745	-499.22	-489.62		741	4	uH = 2.82, d/s = -0.2, h = 0.36
22.29	-	2.0	805 795	-500.06	-490.43		788	6	

218)  $3fa + O_2 = 3q + 2mt$  (Chou, 1978)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
45.08	-	2.0	605 595	-528.65	-519.25	1	606	4	3 (-528.78 <-> -521.82)
41.65	-	2.0	655 645	-529.09	-519.80		655	4	cH = -529.08 (sd 0.95) 2
38.59	-	2.0	705 695	-529.60	-520.34		704	4	too low but OK
36.01	-	2.0	755 745	-531.69	-522.41		749	4	uH = 2.49, d/s = 1.3, h = 0.06
33.41	-	2.0	805 795	-531.38	-522.09		800	4	

219)  $3fa + O_2 = 3q + 2mt$  (Myers & Eugster, 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
41.85	-	0.0	666 656	-532.05	-520.90		660	4	1 (-528.55 <-> -521.52)
38.55	-	0.0	716 706	-530.37	-519.20		713	4	cH = -529.08 (sd 0.95) 2
38.09	-	0.0	721 711	-529.05	-517.84		721	4	too low but OK
36.63	-	0.0	750 740	-530.44	-519.22		747	4	uH = 2.33, d/s = 1.7, h = 0.06
35.77	-	0.0	770 760	-532.32	-521.03		763	4	
21.81	-	0.0	1123 1113	-531.77	-519.33		1115	6	
21.33	-	0.0	1138 1128	-531.21	-518.74		1132	6	

220)  $3fa + O_2 = 3q + 2mt$  (Hewitt, 1978)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
42.64	-	1.0	657 647	-535.68	-526.80		644	4	1 (-532.81 <-> -526.95)
39.08	-	1.0	709 699	-533.42	-525.98		700	4	cH = -529.08 (sd 0.95)
36.26	-	1.0	757 747	-532.69	-527.07		749	4	within bracket
31.25	-	2.0	857 847	-533.84	-526.20		846	4	uH = 2.31, d/s = 1.2, h = 0.25

221) 3fa + O2 = 3q + 2mt (O'Neill, 1987)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
37.98	-	0.0	732	722	-533.37	-526.61		723	4	3 (-531.99 <-> -526.76)
32.77	-	0.0	832	822	-533.17	-526.66		823	4	cH = -529.08 (sd 0.95)
28.43	-	0.0	932	922	-532.94	-526.59		922	4	within bracket
24.74	-	0.0	1032	1022	-532.51	-526.26		1023	6	uH = 1.92, d/s = 1.4, h = 0.42
21.56	-	0.0	1132	1122	-531.88	-525.69		1124	6	

222) q + 2iron + O2 = fa (O'Neill, 1987)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
50.76	-	0.0	732	722	-570.72	-563.05		726	2	1 (-569.60 <-> -563.36)
44.56	-	0.0	832	822	-570.58	-563.22		826	2	cH = -567.34 (sd 0.68)
39.38	-	0.0	932	922	-570.28	-563.22		926	2	within bracket
35.00	-	0.0	1032	1022	-569.95	-563.02		1026	4	uH = 2.29, d/s = 1.4, h = 0.16
31.26	-	0.0	1132	1122	-569.74	-562.92		1126	4	

223) 3iron + 2O2 = mt (O'Neill, 1988)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
138.74	-	0.0	482	472	-1123.92	-1106.36		476	2	1 (-1123.82 <-> -1107.05)
127.80	-	0.0	532	522	-1123.75	-1106.90		526	2	cH = -1115.55 (sd 0.98)
121.32	-	0.0	565	555	-1123.62	-1107.24		559	2	within bracket
										uH = 6.54, d/s = 1.3, h = 0.03

224) 2gth = hem + H2O (Voigt & Will, 1981)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	10.0	180	200	55.63	56.45		184	4	3 (55.46 <-> 56.07)
0	0	20.0	250	280	55.00	56.23		269	4	cH = 55.77 (sd 0.22)
0	0	30.0	300	350	54.55	56.53		331	6	within bracket
0	0	40.0	350	400	54.74	56.43		379	10	uH = 0.22, d/s = 0.7, h = 1.00
0	0	50.0	400	420	55.20	55.95		415	12	

225) sid + hem = mt + CO2 (Koziol, pers com 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	1	6.0	510	520	77.25	78.30		519	6	3 (77.45 <-> 78.94)
0	1	8.0	550	570	77.10	79.23		560	6	cH = 78.17 (sd 0.36)
0	1	9.0	570	590	77.23	79.41		579	6	within bracket
0	1	10.0	590	600	77.51	78.60		596	6	uH = 0.63, d/s = 0.1, h = 0.90
0	1	11.0	600	620	76.78	78.92		613	6	
0	1	12.0	630	640	78.23	79.29	-1	629	6	

226) 2grun = 7fs + 2q + 2H2O (Lattard & Evans, 1992)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	16.0	599		200.11			604	20	6 (199.59 <-> 201.42)
0	0	12.0		637		200.57	1	638	18	cH = 200.69 (sd 1.06)
0	0	14.0	620		200.45			622	20	within bracket
0	0	20.0	563	588	200.58	203.21		564	22	uH = 0.66, d/s = -0.0, h = 0.70

227) 2grun = 7fa + 9q + 2H2O (Lattard & Evans, 1992)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	549	573	196.51	200.76		559	12	1 (196.94 <-> 200.33)
										cH = 198.22 (sd 1.07)
										within bracket
										uH = 0.89, d/s = 2.4, h = 0.31

228) 2deer = 9fs + 6mt + 6q + 10H2O (Lattard & Le Breton, 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	20.0	600	626	609.47	621.94		625	16	2 (616.47 <-> 626.43)
0	0	27.0	710	740	620.96	634.50		711	18	cH = 621.42 (sd 3.62)
										within bracket
										uH = 3.57, d/s = 0.1, h = 0.65

229) deer + Ni = 6fs + 2mt + NiO + 5H2O (Lattard & Le Breton, 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	21.5	570		328.60			604	18	2 (334.32 <-> 338.31)
0	0	20.0		600		338.33		591	16	cH = 336.34 (sd 1.84)
0	0	27.0	640	670	334.29	340.83		649	18	within bracket
										uH = 1.43, d/s = 1.4, h = 0.37

## FeO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

230)  $alm + 3hem = 3mt + ky + 2q$  (Harlov & Newton, 1992)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	23.0	20.0	650	-23.89	-18.71	21.14	0.66	3 (-21.79 <-> -19.75)
0	-	22.5	22.0	700	-20.43	-19.57	0.15	22.65	0.66 cH = -20.69 (sd 0.54)
0	-	26.0	25.5	800	-21.59	-20.73	-0.02	25.48	0.66 within bracket
0	-	29.0	28.0	900	-21.85	-20.12	28.33	0.66	uH = 0.86, d/s = -0.2, h = 0.84

231)  $alm + 2sill = 3herc + 5q$  (Bohlen et al., 1986)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	3.0	800		6.65		708	24	5 (2.49 <-> 3.98)
0	-	2.9	780		6.19		701	26	cH = 3.48 (sd 0.42) 2
0	-	5.2	865 880	3.61	4.17	-4	861	22	within bracket
0	-	5.5	5.1	880	3.44	4.41	5.48	0.43	uH = 0.39, d/s = -2.8, h = 0.82
0	-	6.9	6.5	940	2.31	3.27	-0.09	6.41	0.43
0	-	8.9	8.5	1020	0.63	1.59	-0.79	7.71	0.43
0	-	8.8	1015 1035	0.67	1.47	50	1085	20	

232)  $alm + 5cor = 3herc + 3sill$  (Shulsters & Bohlen, 1989)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	7.2	850	6.73		-58	792	24	6 (4.75 <-> 6.10)
0	-	8.3	7.9	900	5.80	6.91	0.51	8.81	0.34 cH = 4.38 (sd 0.46) 2
0	-	10.6	9.9	1000	3.96	5.88	10.45	0.34	too low but OK
0	-	12.3	11.9	1100	4.15	5.24	12.21	0.35	uH = 0.57, d/s = -1.3, h = 0.24

233)  $2alm + 4sill + 5q = 3fcrd$  (Mukhopadhyay et al., 1991)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	2.3	1.9	650	110.62	115.18	-0.05	1.85	0.14 3 (114.71 <-> 116.75)
0	-	2.5	2.1	700	113.45	117.99	2.30	0.14	cH = 115.71 (sd 1.13)
0	-	2.7	2.3	750	116.30	120.83	0.05	2.75	0.14 within bracket
									uH = 0.73, d/s = -0.8, h = 0.94

234)  $6fst + 25q = 8alm + 46ky + 12H_2O$  (Rao & Johannes, 1979)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	6.0	680 700	998.55	1010.01		683	18	3 (999.59 <-> 1007.87)
0	0	10.0	640 660	993.15	1003.57		654	20	cH = 1000.50 (sd 5.16) 2
0	0	15.0	590 610	1001.23	1010.53	-2	588	24	within bracket
									uH = 3.01, d/s = 0.4, h = 0.75

\*  $6fst + 25q = 8alm + 46ky + 12H_2O$  (Ganguly, 1972)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	7.0	700	1012.49		-21	679	18	** NOT USED **
0	0	10.0	690		1019.16		654	20	cH = 1000.50 (sd 5.16)
0	0	10.6	14.0	650	1001.66	1022.48	-0.21	10.39	2.40
0	0	15.5	600 650	1009.52	1032.50	-20	580	24	

\*  $2fst + 15q = 4fcrd + 10sill + 4H_2O$  (Richardson, 1968)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	550 575	578.35	592.31	12	587	8	** NOT USED **
0	0	4.0	675	596.84			679	8	cH = 598.77 (sd 2.42)
0	0	3.0	650		607.86		633	8	

235)  $23fctd + 7q = 2fst + 5alm + 19H_2O$  (Rao & Johannes, 1979)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.18	0	10.0	560 580	1750.60	1775.69		573	10	2 (1759.19 <-> 1779.14)
1.18	0	14.0	580	1766.25			580	10	cH = 1766.80 (sd 5.92) 2
1.18	0	6.0	560		1772.09		556	10	within bracket
									uH = 7.14, d/s = 0.4, h = 0.06



236) 8fctd + 10ky = 2fst + 3q + 4H2O (Rao & Johannes, 1979)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0.41	0	6.0	530	550	404.48	411.12	-22	508	14	3 (399.29 <-> 404.98)
0.41	0	10.0	550	570	398.84	405.31	-6	544	14	cH = 397.04 (sd 2.38) 2
0.41	0	14.0	570	590	396.09	402.50		573	16	too low but OK
										uH = 2.04, d/s = -0.5, h = 0.38

237) 3fctd = alm + 2cor + 3H2O (Ganguly, 1969; Vidal et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.49	0	12.0	570	595	281.44	286.62	7	602	8	3 (285.83 <-> 288.42)
-0.49	0	19.0	612	640	285.78	291.29		624	8	cH = 288.07 (sd 0.79) 2
-0.49	0	25.0	627	635	287.04	288.58		632	8	within bracket
-0.49	0	30.0	615	650	284.34	290.95		635	10	uH = 1.10, d/s = -0.2, h = 0.16

238) 3fctd = alm + 2cor + 3H2O (Ganguly, 1969)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	8.0	580	600	284.34	288.56		598	8	3 (286.21 <-> 289.04)
0	0	11.5	605	620	285.58	288.63		617	8	cH = 288.07 (sd 0.79) 2
0	0	15.0	620	640	285.84	289.78		631	8	within bracket
0	0	20.0	650	670	289.10	292.93	-5	645	8	uH = 1.02, d/s = -0.3, h = 0.19

239) 3fctd = 4dsp + alm + H2O (Vidal et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
-0.16	0	30.0	615	635	122.80	124.03	7	642	28	2 (122.82 <-> 124.28)
-0.16	0	33.0	580	615	123.06	125.19		603	30	cH = 124.46 (sd 0.81) 2
										too high but OK
										uH = 0.61, d/s = 0.8, h = 0.40

\* 6fst + 25q = 8alm + 46sill + 12H2O (Richardson, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	2.0	680			1481.77		560	10	** NOT USED **
0	0	5.0	675	700	1389.57	1417.82	-49	626	10	cH = 1333.44 (sd 5.68)

240) 6fst + 25q = 8alm + 46sill + 12H2O (Dutrow & Holdaway, 1989)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
7.22	0	3.2	627	647	1324.72	1347.16		635	10	2 (1330.48 <-> 1347.16)
7.22	0	5.0	673	693	1330.48	1351.94		676	10	cH = 1333.44 (sd 5.68) 2
										within bracket
										uH = 5.97, d/s = 1.4, h = 0.14

\* 8fctd + 10sill = 2fst + 3q + 4H2O (Richardson, 1968)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0.41	0	2.0	500	550	330.40	342.42	-24	476	20	** NOT USED **
0.41	0	5.0	525	550	338.40	343.80	-63	462	22	cH = 324.66 (sd 2.47)

\* 5fctd = fcrd + 3herc + 5H2O (Grieve & Fawcett, 1974)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	525	550	529.32	541.94	-13	512	6	** NOT USED **
0	0	2.0	550	575	526.71	538.51	-8	542	6	cH = 522.77 (sd 1.44)

## Na<sub>2</sub>O–FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub> & K<sub>2</sub>O–FeO–Al<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub>

241) 2fgl = 4abh + 3fa + q + 2H<sub>2</sub>O (Hoffmann, 1972)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	3.0	340	370	247.91	257.62		351	28	2 (243.13 <-> 247.91)
0	0	5.0	350	370	236.77	243.14	27	397	30	cH = 251.49 (sd 5.22) 3 too high but OK uH = 1.71, d/s = -1.4, h = 0.47

242) rieb + 3hem = 2acm + 3mt + 4q + H<sub>2</sub>O (Ernst, 1962)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0	0.5	465	490	104.46	108.10		485	8	3 (106.57 <-> 108.18)
0	0	1.0	489	499	106.48	107.86		495	8	cH = 107.38 (sd 0.56)
0	0	2.0	511	516	107.71	108.38	-2	509	8	within bracket uH = 0.68, d/s = 0.1, h = 1.00

\* 2ann + 6sill + 9q = 3fcrd + 2san + 2H<sub>2</sub>O (Holdaway & Lee, 1977)

ln_K	x(CO <sub>2</sub> )	P(kbar)		T(C)		H(low)	H(high)	miss	calc	2sd	summary
1.60	0	2.1	1.9	640		270.85	273.32	-0.30	1.60	0.29	** NOT USED **
1.60	0	2.8	2.6	710		276.20	278.60		2.72	0.31	cH = 277.19 (sd 2.70)

## CaO-FeO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>

\*  $gr + 2alm = 3fa + 3an$  (Bohlen et al., 1983)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.32	-	5.1 4.7	750	34.98	38.38		4.95	0.38	** NOT USED **
5.32	-	5.2 4.8	800	37.99	41.39	0.20	5.40	0.38	cH = 36.25 (sd 1.62)
5.32	-	5.6 5.2	850	38.46	41.86	0.26	5.86	0.39	
5.32	-	6.0 5.6	900	38.95	42.34	0.32	6.32	0.39	
5.32	-	6.4 6.0	950	39.44	42.83	0.38	6.78	0.39	
5.32	-	6.8 6.4	1000	39.96	43.34	0.44	7.24	0.39	
5.32	-	7.1 6.7	1050	41.35	44.73	0.60	7.70	0.39	

\*  $gr + 2alm = 3fa + 3an$  (Perkins & Vielzeuf, 1992)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.32	-	6.4 6.0	900	35.56	38.95		6.32	0.39	** NOT USED **
5.32	-	6.8 6.3	950	36.06	40.29		6.78	0.39	cH = 36.25 (sd 1.62)
5.32	-	7.1 6.6	1000	37.43	41.65	0.14	7.24	0.39	
5.32	-	7.3 7.0	1050	39.66	42.19	0.40	7.70	0.39	

243)  $2hed = 2wo + fa + q$  (Lindsley & Munoz, 1969)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-2.10	-	1.0	945	28.89	33.14		-2.11	0.26	1 (29.33 <-> 32.69)
									cH = 31.11 (sd 1.34) 3
									within bracket
									uH = 0.59, d/s = 3.6, h = 0.05

244)  $2fact = 3fa + 5q + 4hed + 2H_2O$  (Ernst, 1966)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0	1.0	452 465	167.10	169.16	28	493	16	4 (172.35 <-> 174.89)
0	0	2.0	498 509	172.79	174.45		503	18	cH = 173.61 (sd 1.33) 2
0	0	3.0	528 546	176.26	178.90	-18	510	18	within bracket
									uH = 0.76, d/s = -4.6, h = 0.98

245)  $andr = 3pswo + hem$  (Huckenholz & Yoder, 1971)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1130 1150	58.92	59.93		1139	16	1 (59.00 <-> 59.84)
									cH = 59.35 (sd 0.38) 2
									within bracket
									uH = 0.25, d/s = 2.0, h = 0.16

246)  $6andr + 3fa = 6mt + 18wo + 3q$  (Gustavson, 1974)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.5	740 760	203.48	210.61		743	12	3 (203.43 <-> 207.96)
0	-	1.0	760 773	204.04	208.68		761	12	cH = 204.47 (sd 2.13) 2
0	-	2.0	785 797	199.86	204.14	1	798	12	within bracket
									uH = 1.83, d/s = 0.0, h = 0.42

247)  $6andr + 2Ni = 4mt + 18wo + 2NiO$  (Gustavson, 1974)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.5	785 800	253.88	259.09		787	12	3 (252.30 <-> 257.15)
0	-	1.0	795 815	251.37	258.32		805	12	cH = 254.67 (sd 2.13) 2
0	-	2.0	825 840	249.85	255.06		839	12	within bracket
									uH = 1.77, d/s = 0.3, h = 0.40

248)  $6andr = 4mt + 18wo + O_2$  (Moecher & Chou, 1990)

ln_K	x(CO <sub>2</sub> )	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-29.84	-	2.0	840 860	733.21	739.89		840	6	2 (732.02 <-> 741.08)
									cH = 733.56 (sd 2.10) 2
									within bracket
									uH = 3.84, d/s = 0.9, h = 0.05

\* 3andr + mt + 9q = 9hed + 2O2 (Burton et al., 1982)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-82.83	-	2.0	600	1038.02	1046.04	-2.43	-79.85	1.74	** NOT USED **
-68.58	-	2.0	700	1036.81	1045.76	-2.03	-66.00	1.56	cH = 1020.39 (sd 6.30)
-56.97	-	2.0	800	1035.43	1045.60	-1.68	-54.72	1.41	

\* 2andr + q + 3fa = 4hed + 2wo + 2mt (Liou, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.5	540 560	31.33	33.01	-530	10	254	** NOT USED **
0	-	2.0	595 615	33.78	35.70	-499	96	188	cH = 5.93 (sd 2.77)

\* 2andr + 4q + 2Ni = 4hed + 2wo + 2NiO (Liou, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.5	610 650	73.89	77.37	-199	411	64	** NOT USED **
0	-	2.0	670 690	78.39	80.13	-250	420	64	cH = 56.13 (sd 2.92)

\* 3andr + mt + 9q = 9hed + 2O2 (Moecher & Chou, 1990)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-80.87	-	2.0	650	1068.00	1100.51	-6.20	-72.55	1.64	** NOT USED **
-72.99	-	2.0	700	1067.66	1086.29	-5.84	-66.00	1.56	cH = 1020.39 (sd 6.30)

\* 2andr + 4q = 4hed + 2wo + O2 (Moecher & Chou, 1990)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-44.60	-	2.0	600	544.83	568.56	-1.35	-41.61	0.79	** NOT USED **
-40.03	-	2.0	650	550.25	556.08	-1.99	-37.67	0.74	cH = 535.01 (sd 2.86)
-36.38	-	2.0	700	546.38	560.17	-1.41	-34.12	0.71	
-28.85	-	2.0	800	537.30	547.57	-0.26	-28.02	0.64	

\* 3cc + hem + 3q = andr + 3CO2 (Taylor & Liou, 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	2.0	649		240.84		607	6	** NOT USED **
0	0.50	2.0	589 600	241.15	243.65	-38	551	6	cH = 232.36 (sd 0.71)
0	0.22	2.0	550 570	242.94	248.09	-41	509	6	

249) 3q + 2hem + 3gr = 2andr + 3an (Liou, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
7.29	-	3.0	670 694	80.67	82.53	-13	657	26	1 (80.62 <-> 82.57) cH = 79.66 (sd 1.06) 2 too low but OK uH = 0.78, d/s = 1.2, h = 0.23

250) 3gr + 4hem + 5q + 2H2O = 4fep + an (Liou, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.67	0	3.0	670 694	30.16	31.78		680	60	2 (29.95 <-> 31.99) cH = 30.89 (sd 2.02) 3 within bracket uH = 0.87, d/s = 0.9, h = 0.35

251) 3gr + 4hem + 5q + 2H2O = 4fep + an (Holdaway, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.67	0	3.0	690 710	31.52	32.81	-10	680	60	2 (31.14 <-> 33.19) cH = 30.89 (sd 2.02) 3 too low but OK uH = 0.87, d/s = 0.7, h = 0.39

252) 2fep = andr + an + hem + q + H2O (Holdaway, 1972)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.93	0	3.0	690 710	24.38	26.40		692	480	1 (24.59 <-> 26.19) cH = 24.39 (sd 1.07) 3 too low but OK uH = 0.41, d/s = 2.5, h = 0.15

253) 2fep = andr + an + hem + q + H2O (Liou, 1973)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.93	0	3.0	670 694	24.31	26.29		692	480	1 (24.51 <-> 26.08) cH = 24.39 (sd 1.07) 3 too low but OK uH = 0.40, d/s = 2.5, h = 0.16

## Osumilite + KFMASH melt equilibria

\*  $\text{osml} = \text{crd} + \text{san} + 2\text{q}$  (Olesch & Seifert, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.76	-	0.5	760 780	15.96	16.24	124	904	206	** NOT USED **
									cH = 18.17 (sd 2.01) 2

\*  $4\text{phl} + 3\text{crd} + 2\text{san} + 33\text{q} = 6\text{osm2} + 4\text{H2O}$  (Olesch & Seifert, 1981)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-5.88	0	0.5	760 780	536.06	544.19	-24	736	74	** NOT USED **
									cH = 526.11 (sd 14.38) 2

254)  $\text{en} + \text{san} + 2\text{sill} + 3\text{q} = \text{osml}$  (Carrington & Harley, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.13	-	8.3 7.7	900	-9.86	-7.91		8.00	1.11	1 (-9.76 <-> -8.02)
									cH = -8.89 (sd 1.98) 2
									within bracket
									uH = 0.59, d/s = 1.7, h = 1.00

255)  $\text{py} + \text{osm2} = \text{osml} + 2\text{en}$  (Carrington & Harley, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.12	-	8.3 7.7	900	-54.28	-53.87		8.00	3.59	2 (-54.73 <-> -53.41)
									cH = -54.07 (sd 1.24) 2
									within bracket
									uH = 0.56, d/s = 0.4, h = 1.00

256)  $\text{osml} + \text{fs} = \text{fosl} + \text{en}$  (Holland et al., 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.58	-	5.0	825 925	17.36	19.00		864	116	1 (17.50 <-> 18.85)
									cH = 17.99 (sd 0.96) 2
									within bracket
									uH = 0.39, d/s = 2.1, h = 0.39

257)  $\text{fosl} + \text{crd} = \text{osml} + \text{fcrd}$  (Holland et al., 1996)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	5.0	825 925	7.36	8.02		863	260	2 (7.24 <-> 8.14)
									cH = 7.61 (sd 0.85) 2
									within bracket
									uH = 0.38, d/s = 0.9, h = 0.75

258)  $2\text{sill} + 38\text{q} + \text{en} + 12\text{san} = 4\text{mliq}$  (Carrington & Harley, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-12.26	-	8.6	885 895	-1983.56	-1976.79		890	16	2 (-1985.64 <-> -1974.72)
									cH = -1980.17 (sd 5.71)
									within bracket
									uH = 4.64, d/s = 0.7, h = 1.00

259)  $\text{en} + 4\text{fliq} = \text{fs} + 4\text{mliq}$  (Carrington & Harley, 1995)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-2.83	-	8.6	885 895	-33.92	-33.79		891	172	2 (-35.18 <-> -32.52)
									cH = -33.84 (sd 1.16)
									within bracket
									uH = 1.13, d/s = 0.1, h = 1.00

260) hliq = H2O (Carrington & Harley, 1995)

ln_K	x(CO2)	P(kbar)		T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.71	0	8.8	8.4	890	-21.35	-21.12		8.60	2.21	2 (-21.58 <-> -20.89)
										cH = -21.23 (sd 0.65) 2
										within bracket
										uH = 0.29, d/s = 0.4, h = 1.00

## Ni-Ti-Zr-bearing equilibria

261) mag + ru = geik + CO2 (Haselton et al., 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
0	1	13.7	12.7	950	92.52	94.31	-0.29	12.41	0.60	3 (94.05 <-> 95.66)
0	1	19.5	18.5	1100	94.12	95.64		19.02	0.73	cH = 94.85 (sd 0.55)
0	1	26.4	25.4	1250	94.71	96.03		26.29	0.85	within bracket
										uH = 0.68, d/s = -0.3, h = 1.00

262) sph + ky = an + ru (Manning & Bohlen, 1991)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
0	-	15.9	15.5	900	11.23	11.98	0.12	16.02	0.38	3 (10.21 <-> 11.84)
0	-	18.0	17.6	1000	10.79	11.54		17.88	0.39	cH = 11.00 (sd 0.36)
0	-	19.1	18.7	1050	10.50	11.24		18.83	0.39	within bracket
0	-	20.3	19.9	1100	10.03	10.77	-0.12	19.78	0.39	uH = 0.69, d/s = -0.3, h = 0.79

\* ru + cc + q = sph + CO2 (Hunt & Kerrick, 1977; Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.50	2.0	490	510	76.04	77.78	-29	461	10	** NOT USED **
0	0.50	3.5	525	545	74.71	76.34	-14	511	10	cH = 73.55 (sd 0.43)
0	0.78	2.0	510	530	75.63	77.27	-25	485	10	
0	0.50	5.0		580		75.56		554	12	
0	0.97	5.0		635		75.71		604	12	

263) ru + cc + q = sph + CO2 (Jacobs & Kerrick, 1981)

ln_K	x(CO2)	P(kbar)	T(C)		H(low)	H(high)	miss	calc	2sd	summary
0	0.25	6.0	540	560	73.01	74.70		546	10	3 (73.15 <-> 74.14)
0	0.48	6.0	570	580	73.09	73.85		576	12	cH = 73.55 (sd 0.43) 2
0	0.65	6.0	590	610	73.20	74.65		595	12	within bracket
0	0.82	6.0	610	630	73.25	74.65		614	12	uH = 0.42, d/s = 0.7, h = 0.40

264) 2ilm = 2iron + 2ru + O2 (O'Neill et al., 1988)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-48.06	-	0.0	800	573.91	575.64		-47.98	0.16	3 (570.57 <-> 576.45)
-42.52	-	0.0	900	573.40	574.63		-42.53	0.15	cH = 574.11 (sd 0.73)
-40.10	-	0.0	950	573.12	574.34		-40.14	0.14	within bracket
									uH = 2.50, d/s = 0.1, h = 0.23

265) 2ilm = 2iron + 2ru + O2 (Anovitz et al., 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-37.88	-	0.0	1000	569.78	577.10		-37.94	0.14	3 (569.86 <-> 575.80)
-36.72	-	0.0	1025	568.41	575.90		-36.91	0.14	cH = 574.11 (sd 0.73) 2
-35.81	-	0.0	1050	569.15	576.78		-35.91	0.13	within bracket
-34.88	-	0.0	1075	569.47	577.20		-34.95	0.13	uH = 2.13, d/s = 1.4, h = 0.06
-33.96	-	0.0	1100	569.42	577.28		-34.03	0.13	
-32.93	-	0.0	1125	567.61	575.64		-33.14	0.13	

266) 2usp = 2ilm + 2iron + O2 (O'Neill et al., 1988)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-42.29	-	0.0	850	531.46	532.72		-42.32	0.28	3 (529.94 <-> 535.24)
-37.72	-	0.0	950	531.85	533.12		-37.71	0.26	cH = 532.38 (sd 1.30)
-33.85	-	0.0	1050	531.56	533.50		-33.84	0.24	within bracket
									uH = 2.25, d/s = 0.2, h = 0.91

267) 2usp = 2ilm + 2iron + O2 (Anovitz et al., 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-32.01	-	0.0	1100	527.03	534.93		-32.13	0.23	1 (527.62 <-> 532.92)
-30.28	-	0.0	1150	525.11	533.29		-30.55	0.22	cH = 532.38 (sd 1.30) 2
-29.01	-	0.0	1200	527.25	535.70		-29.09	0.21	within bracket
									uH = 1.75, d/s = 1.7, h = 0.09



268)  $\text{alm} + 3\text{ru} = 3\text{ilm} + \text{sill} + 2\text{q}$  (Bohlen et al., 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	11.9 11.4	750	-5.67	-4.71		11.64	0.29	3 (-5.84 <-> -4.54)
0	-	12.4 11.9	800	-5.54	-4.58		12.21	0.29	cH = -5.17 (sd 0.25)
0	-	12.7 12.3	850	-5.00	-4.22	0.09	12.79	0.29	within bracket
0	-	13.4 13.0	900	-5.18	-4.40		13.40	0.29	uH = 0.55, d/s = 0.2, h = 0.99
0	-	14.8 14.4	1000	-5.47	-4.69		14.65	0.29	
0	-	15.5 15.1	1050	-5.60	-4.83		15.28	0.29	
0	-	16.1 15.7	1100	-5.53	-4.76		15.92	0.30	

\*  $2\text{alm} + \text{gr} + 6\text{ru} = 6\text{ilm} + 3\text{an} + 3\text{q}$  (Bohlen & Liotta, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.32	-	10.9 10.5	800	12.30	15.94		10.50	0.18	** NOT USED **
5.32	-	12.3 11.9	900	11.22	14.87	-0.12	11.78	0.18	cH = 15.92 (sd 0.80)
5.32	-	13.5 13.1	1000	12.12	15.75	-0.02	13.08	0.18	
5.32	-	14.5 14.1	1100	14.95	18.56		14.39	0.18	

269)  $\text{zrc} = \text{bdy} + \text{q}$  (Robie et al., 1979)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1665 1685	19.55	19.78		1675	18	1 (19.57 <-> 19.76)
									cH = 19.67 (sd 0.11)
									within bracket
									uH = 0.06, d/s = 2.0, h = 1.00

270)  $2\text{NiO} = 2\text{Ni} + \text{O}_2$  (O'Neill, 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-44.18	-	0.0	600	477.90	481.24		-44.09	0.21	3 (476.43 <-> 482.80)
-32.08	-	0.0	800	477.54	481.63		-32.00	0.17	cH = 478.89 (sd 0.76)
-27.59	-	0.0	900	477.35	481.85		-27.52	0.16	within bracket
-20.59	-	0.0	1100	476.95	482.24		-20.53	0.13	uH = 2.70, d/s = 0.6, h = 0.27

## Exchange equilibria

271) 2mag + fa = fo + 2sid (Dalton & Wood, 1993)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.32	-	20.0	1000	6.06	8.42		-1.25	0.17	1 (6.21 <-> 8.27)
									cH = 6.55 (sd 0.88) 2
									within bracket
									uH = 0.22, d/s = 5.3, h = 0.14

272) 2dol + fa = fo + 2ank (Dalton & Wood, 1993)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.48	-	20.0	1000	10.70	13.47		-1.52	0.49	1 (10.75 <-> 13.42)
									cH = 12.48 (sd 2.58) 2
									within bracket
									uH = 0.22, d/s = 6.4, h = 0.72

\* dol + sid = ank + mag (Anovitz & Essene, 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.35	-	4.0	400	2.00	3.11		-0.42	0.47	** NOT USED **
									cH = 2.97 (sd 1.32) 3

273) dol + sid = ank + mag (Rosenberg, 1967)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.43	-	3.0	500	2.22	4.71		-0.35	0.41	1 (2.41 <-> 4.52)
									cH = 2.97 (sd 1.32) 2
									within bracket
									uH = 0.26, d/s = 4.8, h = 0.30

\* en + 2ank = 2dol + fs (Natural., Klein, 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.80	-	8.0	600	-16.59	-12.92	-1.15	0.40	0.71	** NOT USED **
									cH = -4.60 (sd 2.58) 2

274) py + ann = alm + phl (Ferry & Spear, 1978)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.08	-	2.0	550	-56.36	-54.07		5.11	0.29	1 (-56.18 <-> -54.66)
4.76	-	2.0	600	-58.03	-54.46		4.65	0.27	cH = -55.41 (sd 1.00) 2
4.26	-	2.0	650	-56.64	-54.48		4.24	0.26	within bracket
3.82	-	2.0	700	-56.48	-53.42		3.88	0.25	uH = 0.43, d/s = 2.2, h = 0.80
3.71	-	2.0	745	-58.80	-54.23		3.58	0.24	
3.42	-	2.0	800	-59.48	-54.37		3.25	0.22	

\* py + ann = alm + phl (Perchuk & Lavrenteva, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
3.57	-	6.0	700	-53.69	-49.79	-0.21	4.02	0.25	** NOT USED **
2.97	-	6.0	750	-51.36	-47.27	-0.48	3.69	0.23	cH = -55.41 (sd 1.00)
2.43	-	6.0	800	-49.04	-44.75	-0.71	3.39	0.22	

275) 3fcrd + 2py = 3crd + 2alm (Perchuk & Lavrenteva, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
11.52	-	6.0	700	-145.07	-134.95		11.55	0.38	1 (-141.67 <-> -135.49)
9.73	-	6.0	800	-143.89	-133.16		9.92	0.34	cH = -140.21 (sd 1.54) 2
8.27	-	6.0	900	-143.16	-131.37		8.58	0.32	within bracket
7.03	-	6.0	1000	-142.21	-129.50		7.45	0.29	uH = 0.74, d/s = 4.9, h = 0.05

276)  $alm + 3cel = py + 3fcel$  (Green & Hellman, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.83	-	20.0	975 1025	20.45	21.39		1000	102	1 (20.50 <-> 21.34)
									cH = 20.92 (sd 0.96) 2
									within bracket
									uH = 0.29, d/s = 1.7, h = 1.00

277)  $2hed + en = fs + 2di$  (Lindsley, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.33	-	15.0	990	-12.65	-10.47	-0.25	0.68	0.24	1 (-12.55 <-> -11.76)
0.66	-	15.0	910	-16.94	-10.93		0.80	0.26	cH = -15.26 (sd 1.27) 3
0.68	-	15.0	810	-13.78	-11.65	-0.16	0.96	0.28	too low
									uH = 0.21, d/s = 2.4, h = 0.32

278)  $2hed + fo = fa + 2di$  (Perkins & Vielzeuf, 1992)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.60	-	10.5	1000	-25.59	-21.81		1.55	0.24	1 (-25.25 <-> -22.15)
									cH = -23.14 (sd 1.27)
									within bracket
									uH = 0.44, d/s = 4.3, h = 0.52

\*  $fs + fo = en + fa$  (Matsui & Nishizawa, 1974)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.75	-	27.0	1000	-5.63	-3.17	-0.21	1.08	0.03	** NOT USED **
									cH = -7.88 (sd 0.13) 2

279)  $fs + fo = en + fa$  (von Seckendorff & O'Neill, 1993)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0.94	-	15.0	900	-8.21	-6.71		0.99	0.03	1 (-7.75 <-> -6.83)
0.88	-	15.0	1000	-7.96	-6.68		0.93	0.03	cH = -7.88 (sd 0.13) 2
0.80	-	15.0	1150	-7.88	-6.30	-0.00	0.87	0.02	too low but OK
									uH = 0.22, d/s = 2.6, h = 0.03

280)  $2py + 3fa = 2alm + 3fo$  (O'Neill & Wood, 1979)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.04	-	27.0	1000	-44.10	-37.67		1.93	0.29	1 (-43.69 <-> -39.30)
1.74	-	27.0	1100	-45.02	-37.98		1.58	0.27	cH = -39.74 (sd 1.55) 2
1.49	-	27.0	1200	-45.89	-38.69		1.28	0.25	within bracket
1.25	-	27.0	1300	-46.69	-38.88		1.02	0.24	uH = 0.55, d/s = 4.7, h = 0.16

281)  $2py + 3fa = 2alm + 3fo$  (Hackler & Wood, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.20	-	9.1	1000	-42.39	-35.86		1.26	0.29	1 (-42.42 <-> -35.83)
									cH = -39.74 (sd 1.55) 2
									within bracket
									uH = 0.46, d/s = 7.1, h = 0.04

\*  $2py + 3fs = 2alm + 3en$  (Lee & Ganguly, 1988)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
4.71	-	20.0	980	-68.64	-57.15		4.76	0.29	** NOT USED **
4.43	-	25.0	1055	-66.18	-53.44		4.75	0.28	cH = -63.39 (sd 1.53)
4.25	-	25.0	1105	-67.04	-53.46		4.52	0.27	
3.66	-	25.0	1205	-65.02	-50.68		4.11	0.25	

\*  $2py + 3fs = 2alm + 3en$  (Kawasaki & Matsui, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
5.04	-	45.0	1100	-57.15	-49.51	-0.55	5.92	0.27	** NOT USED **
4.04	-	45.0	1300	-55.08	-45.28	-0.64	5.05	0.23	cH = -63.39 (sd 1.53)

\* 2py + 3fs = 2alm + 3en (Harley, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.98	-	27.0	1200	-54.73	-40.51	-0.71	4.26	0.25	** NOT USED **
2.80	-	23.0	1200	-55.70	-41.81	-0.63	3.99	0.25	cH = -63.39 (sd 1.53)
2.98	-	18.0	1150	-60.02	-46.29	-0.28	3.84	0.26	
3.49	-	18.0	1050	-60.51	-49.08	-0.26	4.27	0.28	
3.99	-	13.5	975	-65.43	-55.15		4.29	0.29	
4.29	-	7.5	900	-68.68	-59.54		4.22	0.31	

\* 2herc + fo = 2sp + fa (Jamieson & Roeder, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.06	-	0.0	1300	0.39	2.19	-0.70	-0.83	0.11	** NOT USED **
									cH = 11.37 (sd 0.71) 2

\* 2herc + fo = 2sp + fa (Engi, 1983)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-0.60	-	1.0	700	4.80	9.58	-0.22	-1.11	0.17	** NOT USED **
-0.31	-	1.0	800	4.09	6.02	-0.60	-1.01	0.16	cH = 11.37 (sd 0.71)
-0.79	-	1.0	900	4.10	15.69		-0.94	0.14	

282) fa + 2mft = 2mt + fo (Jamieson & Roeder, 1984)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
3.61	-	0.0	1300	-42.10	-47.40		3.53	0.64	2 (-45.06 <-> -44.44)
									cH = -43.64 (sd 4.19) 2
									too high but OK
									uH = 0.27, d/s = -10.0, h = 0.64

283) 3en + 2ann = 2phl + 3fs (Fonarev & Konilov, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.59	-	4.9	700	-50.43	-43.39		2.66	0.58	1 (-48.18 <-> -43.55)
2.01	-	4.9	750	-48.34	-40.49		2.37	0.56	cH = -47.44 (sd 2.36) 2
1.82	-	4.9	800	-48.42	-41.36		2.11	0.53	within bracket
									uH = 0.40, d/s = 6.1, h = 0.18

284) fact + 5di = tr + 5hed (Natural Kd)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	6.0	600	0.10	8.82	-0.89	1.49	0.56	1 (0.92 <-> 8.00)
									cH = -6.34 (sd 2.04) 2
									too low
									uH = 1.05, d/s = 4.2, h = 0.06

285) 7en + 2fanth = 2anth + 7fs (Natural Kd)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	5.0	725	20.19	37.70		0.00	4.16	1 (21.37 <-> 36.52)
									cH = 28.95 (sd 17.26) 2
									within bracket
									uH = 1.71, d/s = 5.1, h = 1.00

286) 3tr + 5gl = 5gl + 3fact (Natural Kd)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	10.0	400	3.20	17.25	-0.83	2.09	4.59	1 (2.88 <-> 17.57)
									cH = -1.46 (sd 12.85) 2
									too low but OK
									uH = 0.93, d/s = 7.5, h = 0.59

287) 2acm + pa + 2q = 3ab + hem + H2O (Natural Tauern)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.16	0	10.0	8.0	450	66.05	74.21	8.99	3.80	1 (66.78 <-> 73.48)
									cH = 70.13 (sd 7.63) 2
									within bracket
									uH = 0.94, d/s = 4.3, h = 1.00

288) 5alm + 3clin = 5py + 3daph (Dickenson & Hewitt, 1986; Laird, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-34.81	-	7.0	450	222.72	244.95		-33.30	2.77	1 (224.14 <-> 236.20)
-31.46	-	7.0	500	218.29	237.62		-30.96	2.59	cH = 224.71 (sd 8.32) 2
-29.98	-	7.0	550	222.04	242.06		-28.91	2.43	within bracket
									uH = 1.81, d/s = 4.1, h = 0.47

289) 5phl + 3daph = 5ann + 3clin (Laird, 1989)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.03	-	6.0	550	49.27	62.64		2.55	2.54	1 (50.00 <-> 61.91)
									cH = 52.36 (sd 8.69) 2
									within bracket
									uH = 1.21, d/s = 5.5, h = 0.41

290) clin + fact = tr + daph (Laird, 1982)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
2.66	-	7.0	420	-26.64	-21.72		2.35	1.07	1 (-26.72 <-> -21.64)
									cH = -22.40 (sd 3.08) 2
									within bracket
									uH = 0.33, d/s = 7.4, h = 0.28

291) 4spr7 + 7fcrd = 4fspr + 7crd (Waters, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
12.75	-	5.5	800	-142.65	-172.89		12.75	10.33	2 (-158.94 <-> -156.59)
									cH = -157.78 (sd 46.09) 2
									within bracket
									uH = 1.00, d/s = -15.1, h = 1.00

292) 3fctd + ta = 3mctd + fta (Chinner & Dixon, 1974; Chopin & Monie, 1984; Miller, 1986)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-7.94	-	20.0	550	50.41	55.17	-53	497	68	5 (44.81 <-> 48.85)
-7.69	-	18.0	470	44.00	49.28		513	70	cH = 46.83 (sd 2.33) 2
-6.97	-	20.0	560	44.39	47.99		601	78	within bracket
									uH = 0.55, d/s = -2.2, h = 1.00

293) mcar + fctd = fcar + mctd (Natural, Seidel & Okrusch, 1977; Theye et al., 1992)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.92	-	7.0	330	9.08	10.60		423	64	5 (10.00 <-> 10.99)
-1.95	-	9.0	320	9.09	10.02	31	411	64	cH = 10.49 (sd 0.49) 2
-2.09	-	10.0	370	10.64	11.64	-9	361	58	within bracket
-2.04	-	17.0	420	11.23	12.21	-46	374	60	uH = 0.24, d/s = -2.6, h = 1.00

294) 5sud + 2daph = 5fsud + 2clin (Theye et al., 1992)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-7.53	-	10.0	375	54.14	58.31		400	92	1 (54.53 <-> 57.92)
									cH = 56.23 (sd 3.86) 2
									within bracket
									uH = 0.95, d/s = 2.2, h = 1.00

## Mn-equilibria

295)  $\text{pxmn} = \text{rhod}$  (Maresch & Mottana, 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	3.0	425 450	0.77	0.80		438	20	1 (0.77 <-> 0.80)
0	-	6.0	475 525	0.76	0.82		493	20	cH = 0.79 (sd 0.01)
0	-	20.0	900		0.96		753	20	within bracket
0	-	25.0	800 900	0.73	0.85		847	20	uH = 0.01, d/s = 2.4, h = 1.00
0	-	30.0	900 1000	0.74	0.86		940	20	

296)  $\text{rhc} + \text{q} = \text{pxmn} + \text{CO2}$  (Peters, 1971)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	0.90	2.0	503 509	84.72	85.31	6	515	14	2 (84.83 <-> 86.06)
0	0.60	2.0	490 503	85.58	86.90		493	14	cH = 85.93 (sd 0.73) 2
									within bracket
									uH = 0.52, d/s = -0.3, h = 0.58

297)  $\text{rhc} = \text{mang} + \text{CO2}$  (Huebner, 1969)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	1.0	699 713	111.37	112.85		709	8	3 (111.75 <-> 113.19)
0	1	1.5	739 757	111.72	113.54		746	8	cH = 112.39 (sd 0.43)
0	1	2.0	770 785	111.84	113.31		776	8	within bracket
									uH = 0.55, d/s = 0.9, h = 0.76

298)  $\text{pxmn} + \text{rhc} = \text{teph} + \text{CO2}$  (Huebner & Eugster, 1968)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	1	2.0	555 570	87.32	88.74		561	14	1 (87.34 <-> 88.71)
									cH = 87.90 (sd 0.71)
									within bracket
									uH = 0.51, d/s = 1.4, h = 0.83

299)  $\text{fo} + 2\text{mang} = \text{teph} + 2\text{per}$  (Wood et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.25	-	0.0	1300	5.08	8.19		-1.26	0.15	1 (5.32 <-> 7.96)
									cH = 6.72 (sd 0.98)
									within bracket
									uH = 0.83, d/s = 1.9, h = 0.43

300)  $2\text{spss} + 3\text{fo} = 2\text{py} + 3\text{teph}$  (Wood et al., 1994)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-5.97	-	27.0	1300	37.97	43.94		-6.15	0.78	1 (38.52 <-> 43.38)
									cH = 43.24 (sd 5.07) 2
									within bracket
									uH = 1.38, d/s = 2.2, h = 0.84

301)  $\text{spss} + 3\text{ilm} = \text{alm} + 3\text{pnt}$  (Pownceby et al., 1987)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-5.55	-	5.0	600	3.29	11.56	-0.60	-4.39	1.75	3 (-0.98 <-> 0.45)
-4.68	-	5.0	700	-3.17	7.15		-4.31	1.57	cH = -1.03 (sd 6.34) 2
-3.93	-	5.0	800	-8.97	1.88		-4.22	1.42	too low but OK
-3.34	-	5.0	900	-14.43	-2.93	-0.19	-4.12	1.30	uH = 0.51, d/s = -6.1, h = 0.80

302)  $\text{phl} + 3\text{mnctd} = \text{mnbi} + 3\text{mctd}$  (Mahar et al., 1997)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-8.95	-	4.5	550	68.82	71.49		-8.95	0.70	1 (69.11 <-> 71.20)
									cH = 70.15 (sd 2.38) 2
									within bracket
									uH = 0.47, d/s = 2.9, h = 1.00

303)	4phl + 3mnst = 4mnbi + 3mst	(Mahar et al., 1997)								
ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
-37.63	-	4.5	550	327.72	337.25		-37.63	2.54	1 (328.67 <-> 336.30)	
									cH = 332.48 (sd 8.70) 2	
									within bracket	
									uH = 2.04, d/s = 2.3, h = 1.00	
304)	2phl + 3mnocrd = 2mnbi + 3crd	(Mahar et al., 1997)								
ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
-7.77	-	4.5	550	63.22	68.95		-7.77	1.78	1 (63.41 <-> 68.76)	
									cH = 66.08 (sd 6.09) 2	
									within bracket	
									uH = 0.47, d/s = 6.1, h = 1.00	
305)	5phl + 3mnchl = 5mnbi + 3clin	(Mahar et al., 1997)								
ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
-0.65	-	4.5	550	25.82	37.34		-0.65	5.22	1 (23.74 <-> 39.42)	
									cH = 31.58 (sd 17.87) 2	
									within bracket	
									uH = 0.51, d/s = 11.2, h = 1.00	
306)	phl + spss = mnbi + py	(Mahar et al., 1997)								
ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary	
-16.63	-	4.5	550	116.91	119.10		-16.63	0.68	1 (116.99 <-> 119.03)	
									cH = 118.01 (sd 2.32) 2	
									within bracket	
									uH = 0.73, d/s = 1.5, h = 1.00	

## Melting equilibria

307) **di = diL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1385 1395	-6.86	-6.03		1386	8	3 (-7.42 <-> -6.16)
0	-	10.0	1510 1530	-7.59	-5.86		1519	8	cH = -6.79 (sd 0.36)
0	-	20.0	1620 1640	-7.65	-5.86		1630	8	within bracket
0	-	30.0	1700 1720	-8.76	-6.94	2	1722	8	uH = 0.53, d/s = -0.1, h = 1.00
0	-	50.0	1860 1880	-7.10	-5.21		1863	8	

308) **abh = abL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1115 1125	0.24	0.76		1117	8	3 (-0.03 <-> 0.65)
0	-	10.0	1230 1250	-0.15	0.91		1239	8	cH = 0.32 (sd 0.20)
0	-	20.0	1310 1330	-0.79	0.29	1	1331	8	within bracket
0	-	30.0	1390 1410	-0.14	0.94		1399	8	uH = 0.29, d/s = 0.1, h = 0.77

309) **san = kspL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1180 1220	-7.84	-5.71		1196	10	3 (-7.37 <-> -6.61)
0	-	20.0	1440 1460	-7.56	-6.54		1451	10	cH = -6.99 (sd 0.27)
0	-	30.0	1515 1535	-7.17	-6.18		1519	10	within bracket
0	-	40.0	1540 1560	-7.72	-6.77		1556	12	uH = 0.27, d/s = 0.7, h = 1.00

310) **en = enL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1550 1570	4.31	6.19		1553	10	3 (3.86 <-> 5.37)
0	-	10.0	1660 1680	3.95	5.88		1667	10	cH = 4.62 (sd 0.44)
0	-	20.0	1750 1770	3.40	5.35		1763	10	within bracket
0	-	30.0	1830 1850	3.28	5.26		1844	8	uH = 0.57, d/s = 0.8, h = 1.00
0	-	50.0	1960 1980	3.48	5.48		1971	8	

311) **crst = qL** (Jackson, 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1716 1736	-17.07	-16.92		1718	30	1 (-17.05 <-> -16.93)
									cH = -17.05 (sd 0.11) 2
									within bracket
									uH = 0.04, d/s = 2.0, h = 0.63

312) **q = qL** (Jackson, 1976)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	7.0	1710 1750	-12.80	-12.45	27	1777	24	3 (-12.42 <-> -12.18)
0	-	10.0	1820 1860	-12.58	-12.20		1860	22	cH = -12.21 (sd 0.11) 2
0	-	15.0	1970 2010	-12.39	-11.97		1987	22	within bracket
0	-	20.0	2100 2140	-12.27	-11.83		2105	20	uH = 0.09, d/s = -1.1, h = 0.37

313) **an = anL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1545 1555	-48.34	-47.73		1548	12	1 (-48.39 <-> -47.67)
									cH = -48.16 (sd 0.37)
									within bracket
									uH = 0.30, d/s = 1.0, h = 0.81

314) **an = anL** (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.51	-	5.0	1220 1240	-49.28	-48.11		1239	12	2 (-49.25 <-> -48.19)
-2.21	-	10.0	1105 1125	-49.29	-48.16		1125	12	cH = -48.16 (sd 0.37) 2
									too high but OK
									uH = 0.38, d/s = 1.5, h = 0.19



315) fo = foL (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1885 1895	9.45	10.30		1887	8	3 (9.12 <-> 10.14)
0	-	10.0	1940 1960	9.07	10.73		1947	8	cH = 9.63 (sd 0.33)
0	-	20.0	1980 2000	7.93	9.56	1	2001	8	within bracket
0	-	30.0	2030 2050	8.02	9.62		2050	8	uH = 0.43, d/s = 0.1, h = 1.00
0	-	50.0	2130 2150	9.15	10.72		2136	8	

316) fa = faL (Clarke, 1966)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1200 1222	41.76	43.44		1216	8	3 (42.38 <-> 43.52)
0	-	10.0	1265 1285	42.12	43.61		1276	8	cH = 42.95 (sd 0.32)
0	-	20.0	1323 1343	42.16	43.60		1334	8	within bracket
0	-	30.0	1380 1400	42.30	43.69		1389	10	uH = 0.42, d/s = 0.9, h = 1.00
0	-	50.0	1490 1510	42.65	43.95		1495	10	

317) sill = sill (estimate)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
0	-	0.0	1700 1710	80.14	80.91		1705	14	1 (80.07 <-> 80.98)
									cH = 80.53 (sd 0.52)
									within bracket
									uH = 0.39, d/s = 1.0, h = 1.00

318) h2oL = H2O (Goldsmith & Jenkins, 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
1.90	0	0.9 0.9	900	22.80	23.56	-0.21	0.64	0.04	6 (25.35 <-> 25.89)
1.43	0	2.2 1.8	820	23.81	24.75	-0.30	1.50	0.13	cH = 25.62 (sd 0.21) 2
1.20	0	3.2 2.8	785	24.80	25.36	-0.17	2.63	0.26	within bracket
1.02	0	4.2 3.8	760	25.70	26.11	0.08	4.28	0.42	uH = 0.23, d/s = -4.8, h = 1.00
0.94	0	5.2 4.8	750	25.64	25.99	0.03	5.23	0.49	
0.87	0	6.2 5.8	735	25.73	26.03	0.14	6.34	0.56	
0.73	0	8.2 7.8	715	25.76	26.03	0.22	8.42	0.64	
0.62	0	11.3 10.7	685	25.24	25.60	-0.03	10.67	0.70	

319) abh = abL (Goldsmith & Jenkins, 1985)

ln_K	x(CO2)	P(kbar)	T(C)	H(low)	H(high)	miss	calc	2sd	summary
-1.16	-	1.0	890 910	-0.23	0.88		900	8	3 (-0.11 <-> 0.84)
-1.68	-	2.0	810 830	-0.55	0.58		825	8	cH = 0.32 (sd 0.20) 2
-2.07	-	3.0	775 795	0.30	1.47		775	6	within bracket
-2.30	-	4.0	750 770	0.21	1.40		752	6	uH = 0.34, d/s = 0.4, h = 0.23
-2.39	-	5.0	740 760	-0.27	0.92		750	6	
-2.56	-	6.0	725 745	-0.25	0.95		735	6	
-2.86	-	8.0	705 725	-0.09	1.14		712	6	
-3.22	-	11.0	675 695	-0.64	0.61		690	6	

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