! REFERENCE FILE CONTAINING PRIMARY DATA FOR OXYGEN ISOTOPE FRACTIONATION FACTORS

!

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! GNERAL DESCRIPTION OF THE FILE:

! >> BLOCK

! column 1: phase1/phase2

! column 2: pure/ssNAME (pure = pure phase,ssNAME = solid solutions)

! column 3: number of block involving the phase

! column 4: code (FIT = fir all the data, SELECT = select only the 1st dataset, TEST = do nothing, just plot for comparison)

! _PRIMARY DATA

! column 1: type (Ex=experimental, Th=theoretical and semi-empirical, Mx=mix, NT=natural samples),

! column 2: Reference

! column 3,4,5: A, B, C

! column 6,7: Tmin(°C) Tmax(°C)

! column 8: Tinc (weighting factor)

! **** experimental data (Temperature, fractionation value, 1 standard deviation of the measurements at the given T)

!

!!!! IMPORTANT: All the calibrations marked with "!" at the beginning of the line have been evaluated for this study, but are not included in the final caluclation.

!!!! All the theoretical calculation are restricted to a T range of 200-900 °C.

!!!! All the experimental/natural calibrations exceeding this range are as well reduced to min. 200 °C or max. 900 °C and marked as "!Reduced T range.".

The original T range is left in the block above for comparison, but it is not anymore used for the calculation.

!!!! ---------- !!!!

!!!! ---------- DO NOT MODIFY THE ORDER OF QUARTZ-WATER-CALCITE BLOCK ---------- !!!!

>> QUARTZ/WATER			PURE			#1	FIT	<<------
_TH_	Zheng(1993a)		4.48	-4.77	1.71	0	900	20
! Theoretical calculation by incremental method.								
_TH_	Richter&Hoernes(1988)		3.70	0.00	-3.21	300	800	20
! Water parameters are taken from experimental data from the literature (not specified).								
! An "average qtz-water curve" forms the basis for the increment method calculation.								
!_EX_	Clayton&al(1972)		3.38	0.00	-3.40	200	500	5
! ! Parameters corrected by Freidman&O'Neil(1977).								
!_EX_	Clayton&al(1972)		2.51	0.00	-1.96	500	750	5
!****	490	2.30	0.06					
!****	550	1.78	0.06					
!****	580	1.54	0.09					
!****	650	0.98	0.21					

!**** 750 0.41 0.21

! ! Parameters corrected by Freidman&O'Neil(1977).

_EX_ Clayton&al(1972) 3.38 0.00 -2.90 200 500 5

! Parameters corrected by Freidman&O'Neil(1977).

_EX_ Clayton&al(1972) 2.51 0.00 -1.46 500 750 5

! Parameters corrected by Freidman&O'Neil(1977).

_MX_ Bottinga&Javoy(1973) 4.10 0.00 -3.70 500 800 5

! Based on exp data from O'Neil and Taylor(1967) + theoretical consideration + natural samples.

! Parameters corrected by Freidman&O'Neil(1977) corresponds to the ones reported here.

_EX_ Matsuhisa&al(1979) 2.05 0.00 -1.14 500 800 5

**** 800 0.64 0.01

**** 700 1.06 0.06

**** 600 1.49 0.23

**** 500 2.31 0.09

_EX_ Matsuhisa&al(1979) 3.13 0.00 -2.94 400 500 5

**** 400 4.11 0.11

_EX_ Matsuhisa&al(1979) 3.34 0.00 -3.31 250 400 5

**** 300 6.64 0.06

**** 250 9.03 0.00

_EX_ Zhang&al(1989) 3.31 0.00 -2.71 180 550 10

! Little salt effect observed.

_EX_ Hu&Clayton(2003) 2.35 0.00 -1.16 400 750 5

_EX_ Sharp&Kirschner(1994) 3.65 0.00 -2.9 200 800 5

! Obtained by combining the quartz-calcite and calcite-water equations (this study and O'Neil&al, 1969).

!_MX_ Shiro&Sakai(1972) 3.55 0.00 -2.57 195 573 5

! ! Parameters reported as corrected by Freidman&O'Neil(1977).

! ! Not considered because based on an oversimplified theory (Z. Sharp, personal communication).

!_MX_ Shiro&Sakai(1972) 3.23 0.00 -2.94 573 1000 5

! ! Parameters reported as corrected by Freidman&O'Neil(1977).

! ! Not considered because based on an oversimplified theory (Z. Sharp, personal communication).

_MX_ Freidman&O'Neil(1977) 3.38 0.00 -2.9 500 750 5

! The given parameters are based on published and unpublished data by Compston&Epstein(1958),Staschewski(1964),Majzoub(1966),O'Neil&Epstein(1966),Bottinga&Craig(1969),Matsuhisa&al(1971),Blattner(1973),Horibe&al(1973),Friedman&Gleason(unpub.data,1974),O'Neil&al(1975),Clayton(unpub.data,1975).

! Reported in Früh-Green&al(1996).

! T range from Clayton&al(1972).

_EX_ Matthwes&Beckinsale(1979) 3.05 0.00 -2.09 265 465 5

**** 265 8.61 0.59
**** 360 5.34 0.30
**** 465 3.61 0.24
! Study on hydrothermal crystallization of quartz at 1.02 kbar.

_MX_ Becker&Clayton(1976) 3.19 0.42 -3.51 0 727 5
! Parameters recalculated by polynomial regression of the point data given in the paper. R^2=0.99999.
! Linear regression: A=3.28, C=-3.10, R^2=0.9999.
! Details on the calculation method in the paper.

!_MX_ Kawabe(1978) 1.3 -0.42 -2.07 0 100 5

_EX_ Kita&al(1985) 3.52 0.00 -4.35 20 120 5
! Obtained by measuring the oxygen isotope ratios of amorphous silica precipitated from geothermal waters of power plants at 34-93 °C.

_NT_ Leclerc&Labey(1987) 3.26 0.45 0.00 0 25 5
! Marine diatom sediment samples. taking into account the exchangeable part of the oxygen in biogenic silica.! ! A = 3.26 ± 0.40, B = 0.45 ± 4.9.

_EX_ Brandriss&al(1998) 0.00 15.56 -20.92 0 20 5
! Freshwater diatom grown in batch cultures at temperatures 3.6-20.0 °C
! Low results with respect to other studies on low T samples)

>> CALCITE/WATER CARBONATE #1 FIT <<------

_TH_ Zheng(1999) 4.01 -4.66 1.71 0 900 20
! Theoretical calculation by incremental method.

_EX_ Kim&O'Neil(1997) 0 18.03 -32.42 10 40 5
**** 10 33.01 0.96
**** 25 28.92 0.56
**** 40 25.85 0.45

_EX_ Hu&Clayton(2003) 2.01 0 -1.77 300 750 5
**** 750 1.14 0.05
**** 600 1.84 0.12
**** 500 2.73 0.10
**** 400 4.10 0.10
! equilibrium fractionation factors calculated on the basis of the method of Northrop&Clayton(1966) and Matsuhisa&al(1979).

!_EX_ O'Neil&al(1969) 2.78 0 -3.39 0 500 5
!**** 700 -0.12 0.02
!**** 500 1.50 0.12
!**** 430 2.33 0.20
!**** 400 2.75 0.15
!**** 370 3.10 0.16
!**** 350 3.56 0.00
!**** 320 4.27 0.18
!**** 240 7.18 0.19
!**** 201 9.41 0.19

!**** 25 27.98 0.08

!**** 0 33.94 0.00

! ! Parameters corrected by Freidman&O'Neil(1977).

_EX_ O’Neil&al(1969) 2.78 0.00 -2.89 0 500 5

! Parameters corrected by Freidman&O'Neil(1977). Few data at low T.

_EX_ Epstein&al(1953) 2.73 0.00 -2.71 7 30 5

_EX_ Northrop&Clayton(1966) 2.70 0.00 -2.00 0 750 5

! Derived by O'Neil(1963).

_NT_ Coplen(2007) 0.00 17.40 -28.6 13 40 5

! Fractionation between ground water and inorganically precipitated Holocene vein calcite from Devils Hole cave.

! Typically higher than other experiments.

_TH_ Horita&Clayton(2007) 0.95 11.59 -21.56 0 100 5

>> QUARTZ/CALCITE CARBONATE #2 TEST <<------

_TH_ Zheng(1999) 0.47 -0.10 0.00 0 900 20

! Theoretical calculation by incremental method.

_EX_ Clayton&al(1989) 0.38 0.00 0.00 600 900 5

**** 1000 0.19 0.1

**** 800 0.32 0.1

**** 700 0.39 0.1

**** 600 0.53 0.1

! StDev estimated from the plot on the original paper.

! Standard error of the coefficient = 0.08 calculated in Chiba&al(1989).

_NT_ Sharp&Kirschner(1994) 0.87 0.00 0.00 100 700 5

_EX_ Clayton&al(1972) 0.60 0.00 0.00 200 500 5

! The authors use their data for qtz-water, and data for cal-water from O'Neil et al (1969) to calculate these parameters.

_EX_ Chacko&al(1996) 0.40 0.00 -0.60 500 800 5

! Parameters obtained by combining data from experiments on different mineral couples.

!!!! ---------- !!!!

!!!! ---------- CARBONATES ---------- !!!!

>> QUARTZ/ANKERITE PURE #1 FIT <<------

!_TH_ Zheng(1999) 0.36 -0.15 0.03 0 900 20

! ! Theoretical calculation by incremental method.

_TH_	Zheng&Boettcher(2016)	0.41	-0.20	0.05	0	900	20	
! Theoretical calculation by incremental method.								
>> ANKERITE/WATER		PURE			#2	TEST		<<------
!_TH_	Zheng(1999)	4.12	-4.62	1.71	0	900	20	
! ! Theoretical calculation by incremental method.								
_TH_	Zheng&Boettcher(2016)	4.07	-4.56	1.69	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/ANKERITE		PURE			#2	TEST		<<------
_TH_	Zheng&Boettcher(2016)	-0.06	-0.10	0.05	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/ARAGONITE		PURE			#1	FIT		<<------
_TH_	Zheng(1999)	0.57	1.03	-0.47	0	900	20	
! Theoretical calculation by incremental method.								
>> ARAGONITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1999)	3.91	-5.79	1.92	0	900	20	
! Theoretical calculation by incremental method.								
_EX_	Kim&al(2007)	0.00	17.88	-31.14	0	40	5	
! Precipitated aragonite.								
_NT_	Patterson&al(1993)	0.00	18.56	-33.49	3	30	5	
! Paired otolith and water samples were analyzed fron six large modern temperate lakes.								
! Uncertainty on B = 0.319, uncertainty on C = 0.307.								
_NT_	Grossman&Ku(1986)	0.00	18.04	-31.12	2	22	5	
! Analyses performed on live and modern specimens of aragonitic foraminifera, gastropods and scaphopods.								
>> AZURITE/WATER		PURE			#1	FIT		<<------
_EX_	Melchiorre&al(2000)	2.67	0.00	4.75	10	45	5	
! Slow precipitation experiments + study on natural samples.								
>> CERUSSITE/WATER		PURE			#1	FIT		<<------
_TH_	Zheng(1999)	3.96	-5.28	1.82	0	900	20	

! Theoretical calculation by incremental method.

! Corrected from Table 4 in the reference paper.

_EX_	Melchiorre&al(2001)			2.63	0.00	-3.58	20	65	5
****	20	27.02	0.5						
****	25	26.01	0.5						
****	30	25.04	0.5						
****	35	24.12	0.5						
****	45	22.40	0.5						
****	50	21.61	0.5						
****	55	20.84	0.5						
****	65	19.42	0.5						

! Slow precipitation experiments + study on natural samples.

! CO2 liberated by acidification corrected as total calcite oxygen.

! there is some uncertainty with regard to the state of equilibrium attained.

>> QUARTZ/CERUSSITE		PURE			#2	TEST	<<------
_TH_	Zheng(1999)	0.52	0.52	-0.25	0	900	20

! Theoretical calculation by incremental method.

>> DOLOMITE/WATER		CARBONATE			#1	FIT	<<------
!_TH_	Zheng(1999)	4.06	-4.65	1.71	0	900	20

! ! Theoretical calculation by incremental method.

_TH_	Zheng&Boettcher(2016)	4.03	-4.64	1.70	0	900	20

! Theoretical calculation by incremental method.

!_EX_	Northrop&Clayton(1966)	3.20	0.00	-2	300	510	5

! ! Direct exchange at P=1kbar.

! ! Parameters corrected by Freidman&O'Neil(1977).

_EX_	Northrop&Clayton(1966)	3.20	0.00	-1.50	300	510	5

! Parameters corrected by Freidman&O'Neil(1977).

_EX_	Matthews&Katz(1977)	3.06	0.00	-3.24	252	295	5

! Hydrothermal dolomitization of calcite or aragonite in presence of Ca-Mg-CO3 solution at P=1 atm.

! The linear correlation coefficient of the regression curve through the experimental values is r = 0.987.

_EX_	Vasconcelos&al(2005)	2.73	0.00	0.26	25	45	5

! Microbial experiments.

_EX_	Horita(2014)	3.14	0.00	-3.14	80	350	5

! Direct precipitation (80 °C) and dolomitization of CaCO3 (100–350 °C).

! 1sigma A = 0.022, 1sigma C = 0.11.

_EX_	Schmidt&al(2005)	2.63	0.00	3.12	40	80	5

! Synthesized carbonate samples.

_EX_	Fritz&Smith(1970)	3.20	0.00	-2.0	25	80	5	

>> QUARTZ/DOLOMITE		CARBONATE			#2	TEST		<<------
!_TH_	Zheng(1999)	0.42	-0.12	0.01	0	900	20	

! ! Theoretical calculation by incremental method.

_TH_	Zheng&Boettcher(2016)	0.45	-0.13	0.01	0	900	20	

! Theoretical calculation by incremental method.

>> CALCITE/DOLOMITE		CARBONATE			#3	TEST		<<------
_TH_	Zheng&Boettcher(2016)	-0.01	-0.02	0.01	0	900	20	

! Theoretical calculation by incremental method.

_EX_	Northrop&Clayton(1966)	-0.5	0.00	0.00	300	510	5	
_NT_	Sheppard&Schwarcz(1970)	-0.45	0.00	0.40	100	650	5	

! Fractionation between coexisting calcite and dolomite in marbles.

_EX_	O'Neil&Epstein(1966)	-0.56	0.00	0.45	350	400	5	

! Based on measurements at only two temperatures (350 and 400 °C).

>> QUARTZ/MAGNESITE		CARBONATE			#1	FIT		<<------
_TH_	Zheng(1999)	0.41	-0.13	0.01	0	900	20	

! Theoretical calculation by incremental method.

>> MAGNESITE/WATER		CARBONATE			#2	TEST		<<------
_TH_	Zheng(1999)	4.07	-4.64	1.72	0	900	20	

! Theoretical calculation by incremental method.

>> MALACHITE/WATER		PURE			#1	FIT		<<------
_EX_	Melchiorre&al(2000)	2.66	0.00	2.66	0	50	5	

! Slow precipitation experiments + study on natural samples.

>> NORSETHITE/WATER		PURE			#1	FIT		<<------
_TH_	Zheng&Boettcher(2016)	3.88	-4.89	1.73	0	900	20	

! Theoretical calculation by incremental method.

! BaMg(CO3)2.

_EX_	Bötcher(2000)	2.83	0.00	-2.85	20	135	5

! Experimental formation of ordered norsethite from the reaction of anhydrous witherite with relatively low concentrated sodium-magnesium bicarbonate solutions.

! Isotope equilibrium was not reached within run time.

>> QUARTZ/NORSETHITE		PURE			#2	TEST	<<------
_TH_	Zheng&Boettcher(2016)	0.60	0.12	-0.10	0	900	20

! Theoretical calculation by incremental method.

>> CALCITE/NORSETHITE		PURE			#3	TEST	<<------
_TH_	Zheng&Boettcher(2016)	0.13	0.23	-0.10	0	900	20

! Theoretical calculation by incremental method.

>> OTAVITE/WATER		PURE			#1	FIT	<<------
_TH_	Zheng(1999)	4.07	-4.64	1.71	0	900	20

! Theoretical calculation by incremental method.

_EX_	Kim&O'Neil(1997)	2.76	0.00	-3.96	0	500	5

****	10	30.54	0.07
****	25	27.20	0.22
****	40	24.32	0.28
****	250	5.97	0.11
****	320	2.95	0.25

! Divalent metal carbonates synthesized over T = 0-40°C by the classical method of slowly bubbling N2 through a bicarbonate solution.

! Combining new data for low-T precipitations (T=10-40°C) and the high-T equilibrium fractionations published by O'Neil&al(1969) (T > 40°C).

! Exp. points are reported with 1SD on all the measurements at the same temperature.

>> QUARTZ/OTAVITE		PURE			#2	TEST	<<------
_TH_	Zheng(1999)	0.41	-0.12	0.01	0	900	20

! Theoretical calculation by incremental method.

>> RHODOCHROSITE/WATER		PURE			#1	FIT	<<------
_TH_	Zheng(1999)	4.19	-4.59	1.72	0	900	20

! Theoretical calculation by incremental method.

_EX_	Kim&al(2009)	2.65	0.00	-0.26	10	40	5

! Rhodochrosite crystals precipitated from Na–Mn–Cl–HCO3 parent solutions following passive, forced and combined passive-to-forced CO2 degassing methods.

! Uncertainty on A = 0.03, uncertainty on C = 0.35.

>> QUARTZ/RHODOCHROSITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.29 -0.17 0.04 0 900 20

! Theoretical calculation by incremental method.

>> SIDERITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1999) 4.23 -4.58 1.73 0 900 20

! Theoretical calculation by incremental method.

_MX_ Becker&Clayton(1976) 2.89 0.00 -2.83 0 727 5

! Parameters recalculated by linear regression of the point data given in the paper. R^2=0.9998.

! The calculation was done by the same methods used for other carbonates by O'Neil&al(1969).

! Polynomial regression option A=2.73, B=0.77, C=-3.59, R^2=0.9998.

_EX_ Carothers&al(1988) 3.13 0.00 -3.50 30 200 5

**** 33 29.88 0.1

**** 56 26.06 0.1

**** 103 18.75 0.1

**** 150 13.18 0.1

**** 197 10.61 0.1

! Synthetic siderite prepared by low addition of ferrous chloride solutions to sodium bicarbonate solutions.

! Comparison between the EX and TH fractionations favorable only at ca.200°C; at lower T they generally differ by up to 2 permil.

_EX_ Zhang&al(2001) 2.56 0.00 1.69 45 75 5

! Experiments were performed by using mesophilic and thermophilic iron-reducing bacteria.

! Oxygen isotope fractionation occurred between biogenic siderite and water from which the mineral was precipitated.

>> QUARTZ/SIDERITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.25 -0.19 0.05 0 900 20

! Theoretical calculation by incremental method.

>> SMITHSONITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1999) 4.27 -4.56 1.73 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/SMITHSONITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.21 -0.2 0.06 0 900 20

! Theoretical calculation by incremental method.

>> STRONTIANITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1999) 3.9 -5.93 1.95 0 900 20

! Theoretical calculation by incremental method.

!_EX_ O'Neil&al(1969) 2.69 0 -3.74 0 500 5

!**** 500 0.97 0.22

!**** 400 1.97 0.22

!**** 370 2.60 0.09

!**** 320 3.87 0.02

!**** 250 6.24 0.20

! ! Experimental method by Clayton2(1961) for equilibrating calcium carbonate and water. Stable polymorphs of the carbonates were used.

! ! Exp. points are reported with 1SD on all the measurements at the same temperature.

! ! Parameters corrected by Freidman&O'Neil(1977).

_EX_ O'Neil&al(1969) 2.69 0 -3.24 0 500 5

! Parameters corrected by Freidman&O'Neil(1977).

>> QUARTZ/STRONTIANITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.58 1.16 -0.52 0 900 20

! Theoretical calculation by incremental method.

>> WITHERITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1999) 3.87 -6.15 1.99 0 900 20

! Theoretical calculation by incremental method.

_EX_ O'Neil&al(1969) 2.57 0 -4.23 0 500 5

**** 500 -0.25 0.20

**** 400 0.3 0.02

**** 370 1.45 0.39

! Experimental method by Clayton2(1961) for equilibrating calcium carbonate and water. Stable polymorphs of the carbonates were used.

! Parameters corrected by Freidman&O'Neil(1977) do not diverge from the ones reorted here.

_EX_ Kim&O'Neil(1997) 2.63 0 -4.04 0 500 5

**** 10 29.81 0.80

**** 25 26.30 0.54

**** 40 23.28 0.41

! Divalent metal carbonates synthesized over T = 0-40°C by the classical method of slowly bubbling N2 through a bicarbonate solution.

! Combining new data for low-T precipitations and the high-T equilibrium fractionations published by O'Neil&al(1969).

! Exp. points are reported with 1SD on all the measurements at the same temperature.

>> QUARTZ/WITHERITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.61 1.38 -0.61 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- FELDSPAR ---------- !!!!

>> ALBITE/WATER FELDSPAR #1 FIT <<------

_TH_ Zheng(1993a) 4.33 -6.15 1.98 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.79 -0.32 -2.83 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Same values for albite and othoclase.

_EX_ O’Neil&Taylor(1967) 2.91 0 -3.41 350 800 10

**** 800 -1.04 0.24

**** 600 0.54 0.16

**** 500 1.51 0.21

**** 420 2.58 0.00

**** 350 3.96 0.16

! ultra-fine high albite/syn. sanidine prepared by reacting natural pegmatitic albite (Amelia, Virginia). Water +- HCl solutions.

! same equation for albite and K-Feld.

! In agreement with corrected data reported in Friedman&O'Neil(1977).

_MX_ Bottinga&Javoy(1973) 3.13 0 -3.70 500 800 5

! Based on exp data from o'Neil and Taylor(1967) + theoretical consideration + natural samples.

! In agreement with corrected data reported in Friedman&O'Neil(1977).

_EX_ Matsuhisa&al(1979) 1.59 0 -1.16 500 700 5

**** 700 0.55 0.08

**** 600 0.86 0.30

_EX_ Matsuhisa&al(1979) 2.39 0 -2.51 400 500 5

**** 500 1.76 1.65

**** 400 2.79 1.61

>> QUARTZ/ALBITE FELDSPAR #2 TEST <<------

_TH_ Zheng(1993a) 0.15 1.39 -0.57 0 900 20

! Theoretical calculation by incremental method.

_EX_ Matsuhisa&al(1979) 0.46 0 0.02 500 800 5

! Calculated by using the Qtz-Water parameters presented in the same paper.

! The equation is given as quartz-feldspar fractionation based on the mole fraction of anorthite. Here An=0.

_EX_ Matsuhisa&al(1979) 0.74 0 -0.43 400 500 5

! Calculated by using the Qtz-Water parameters presented in the same paper.

! The equation is given as quartz-feldspar fractionation based on the mole fraction of anorthite. Here An=0.

_EX_ Matthews&al(1983a) 0.50 0 0 400 800 5

! Pyroxene-water fractionation was experimetally studied. Quartz and feldspar data from Matsuhisa et al (1979).

_EX_ Chiba&al(1989) 0.94 0 0 600 800 5

! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).

! Fractionation data combined with the data of Clayton&al(1989).

! Standard error of the coefficient = 0.10.

>> CALCITE/ALBITE FELDSPAR #3 TEST <<------

_TH_ Zheng(1993a) -0.32 1.49 -0.57 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 0.62 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

_EX_ Chiba&al(1989) 0.56 0 0 600 900 5

! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).

! Fractionation data combined with the data of Clayton&al(1989).

! Standard error of the coefficient = 0.06.

_EX_ Clayton&al(1989) 0.57 0.00 0.00 600 900 5

>> ANORTHITE/WATER FELDSPAR #1 FIT <<------

_TH_ Zheng(1993a) 4.12 -7.5 2.24 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.89 -0.63 -2.46 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Same values for albite and orthoclase.

_EX_ O’Neil&Taylor(1967) 2.15 0 -3.82 500 800 10

**** 800 -2.00 0.00

**** 600 -0.94 0.14

**** 500 -0.29 0.14

**** 420 +0.11 0.00

! In agreement with corrected data reported in Friedman&O'Neil(1977).

_MX_ Bottinga&Javoy(1973) 2.09 0 -3.70 500 800 5

! Based on exp data from o'Neil and Taylor(1967) + theoretical consideration + natural samples.

! In agreement with corrected data reported in Friedman&O'Neil(1977).

_EX_ Matsuhisa&al(1979) 1.04 0 -2.01 500 750 5
**** 750 -1.05 0.09
**** 700 -0.90 0.05
**** 600 -0.67 0.01

_EX_ Matsuhisa&al(1979) 1.49 0 -2.81 400 500 5
**** 500 -0.28 0.11
**** 460 -0.09 0.10
**** 400 -0.50 0.37

>> QUARTZ/ANORTHITE FELDSPAR #2 TEST <<------

_TH_ Zheng(1993a) 0.36 2.73 -1.14 0 900 20
! Theoretical calculation by incremental method.

_EX_ Matsuhisa&al(1979) 1.01 0 0.87 500 800 5
! Calculated by using the Qtz-Water parameters presented in the same paper.
! The equation is given as quartz-feldspar fractionation based on the mole fraction of anorthite. Here An=1.

_EX_ Matsuhisa&al(1979) 1.64 0 -0.73 400 500 5
! Calculated by using the Qtz-Water parameters presented in the same paper.
! The equation is given as quartz-feldspar fractionation based on the mole fraction of anorthite. Here An=1.

_MX_ Javoy&al(1970) 0.62 0 0.77 200 900 5
! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.
! Changed from the original papaer (symmetric fit with respect to x axis).

_EX_ Matthews&al(1983a) 1.59 0 0 400 800 5
! Pyroxene-water fractionation was experimetally studied. Quartz and feldspar data from Matsuhisa et al (1979).

_EX_ Chiba&al(1989) 1.99 0 0 600 800 5
! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).
! Fractionation data combined with the data of Clayton&al(1989).
! Standard error of the coefficient = 0.10.

>> CALCITE/ANORTHITE FELDSPAR #3 TEST <<------

_TH_ Zheng(1993a) -0.11 2.83 -1.14 0 900 20
! Theoretical calculation by incremental method.

_EX_ Chiba&al(1989) 1.61 0 0 600 900 5
! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).
! Fractionation data combined with the data of Clayton&al(1989).
! Standard error of the coefficient = 0.07.

!_TH_ Hoffbauer&al(1994) 1.61 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

_EX_ Clayton&al(1989) 1.59 0.00 0.00 600 900 5

>> KFELDSPAR/WATER FELDSPAR #1 FIT <<------

_TH_ Zheng(1993a) 4.32 -6.27 2 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.79 -0.32 -2.83 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.
! Same values for albite and othoclase.

_EX_ O'Neil&Taylor(1967) 2.91 0 -3.41 500 800 10
**** 800 -1.04 0.24
**** 600 0.54 0.16
**** 500 1.51 0.21
**** 420 2.58 0.00
**** 350 3.96 0.16
! ultra-fine high albite/syn. sanidine prepared by reacting natural pegmatitic albite (Amelia, Virginia). Water +- HCl solutions.
! same equation for albite and K-Feld.

>> QUARTZ/KFELDSPAR FELDSPAR #2 TEST <<------

_TH_ Zheng(1993a) 0.16 1.5 -0.62 0 900 20
! Theoretical calculation by incremental method.

_MX_ Javoy&al(1970) 0.62 0 0.77 200 900 5
! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.
! Changed from the original papaer (symmetric fit with respect to x axis).

>> CALCITE/KFELDSPAR FELDSPAR #3 TEST <<------

_TH_ Zheng(1993a) -0.3 1.6 -0.62 0 900 20
! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 0.62 0 0 600 900 20
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- GARNETS ---------- !!!!

>> QUARTZ/ANDRADITE GARNET #1 FIT <<------

_TH_ Zheng(1993a) 0.72 4.29 -1.8 0 900 20

! Theoretical calculation by incremental method.

>> ANDRADITE/WATER GARNET #2 TEST <<------

_TH_ Zheng(1993a) 3.76 -9.05 2.52 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.88 -0.99 -2.04 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/ANDRADITE GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.26 4.38 -1.8 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.68 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> GROSSULAR/WATER GARNET #1 FIT <<------

_TH_ Zheng(1993a) 3.74 -9.11 2.52 0 900 20

! Theoretical calculation by incremental method.

_MX_ Matthews(1994) -1.70 0 0 600 800 5

**** 800 -1.51 0.25

**** 700 -1.77 0.25

!Linear eqation calculated on the base of the available points (3 point if the inntercept=0 is considered).

_TH_ Richter&Hoernes(1988) 0.73 -1.04 -1.98 300 800 5

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/GROSSULAR GARNET #2 TEST <<------

_TH_ Zheng(1993a) 0.74 4.35 -1.82 0 900 20

! Theoretical calculation by incremental method.

_NT_ Valley&al(2003) 2.71 0 0 500 900 5

! T range is not clearly assigned in the paper.

_MX_ Matthews(1994) 3.03 0 0 600 800 5

!Recalculated using Grs/water from this work and Qtz/water from Bottinga&Javoy(1973).

!_EX_ Chacko&al(2001) 3.15 0 0 800 1200 5

! ! Recalculated from experimental data for Garnet-Calcite of Rosenbaum&Mattey(1995).

_EX_ Chacko&al(2001) 3.15 0 0 800 900 5

! Reduced T range.

>> CALCITE/GROSSULAR GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.27 4.45 -1.82 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.84 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!_EX_ Rosenbaum&Mattey(1995) 2.77 0 0 800 1200 5

! ! Experiments at ca. 23 kbar.

_EX_ Rosenbaum&Mattey(1995) 2.77 0 0 800 900 5

! Reduced T range.

_EX_ Matthews(1994) 2.65 0 0 400 700 5

! Combining min-water data with quartz-water data from Matsuhisa et al (1979).

>> QUARTZ/ALMANDINE GARNET #1 FIT <<------

_TH_ Zheng(1993a) 0.72 4.26 -1.79 0 900 20

! Theoretical calculation by incremental method.

_NT_ Valley&al(2003) 2.71 0 0 500 900 5

**** 725 2.33 0.25

**** 675 2.14 0.26

! point data are from natural samples (Peck et al, 2003). T range is not clearly assigned in the paper.

>> ALMANDINE/WATER GARNET #2 TEST <<------

_TH_ Zheng(1993a) 3.76 -9.02 2.52 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.76 -1.03 -1.99 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/ALMANDINE GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.25 4.36 -1.79 0 900 20

! Theoretical calculation by incremental method.

>> PYROPE/WATER GARNET #1 FIT <<------

_TH_ Zheng(1993a) 3.75 -9.07 2.52 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.73 -1.04 -1.98 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/PYROPE GARNET #2 TEST <<------

_TH_ Zheng(1993a) 0.73 4.3 -1.8 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/PYROPE GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.26 4.41 -1.81 0 900 20
! Theoretical calculation by incremental method.

>> QUARTZ/SPESSARTINE GARNET #1 FIT <<------

_TH_ Zheng(1993a) 0.73 4.31 -1.81 0 900 20
! Theoretical calculation by incremental method.

_EX_ Lichtenstein&Hoernes(1992) 2.83 0 0 500 750 5
! Parameters obtained by combining the sps/H2O fractionation with the qtz/water fractionation from Bottinga&Javoy(1973).

>> SPESSARTINE/WATER GARNET #2 TEST <<------

_TH_ Zheng(1993a) 3.75 -9.07 2.52 0 900 20
! Theoretical calculation by incremental method.

_EX_ Lichtenstein&Hoernes(1992) 1.27 0 -3.65 500 750 5
**** 750 -2.1 0.00

_TH_ Richter&Hoernes(1988) 0.74 -1.04 -1.98 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/SPESSARTINE GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.26 4.41 -1.81 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/UVAROVITE GARNET #1 FIT <<------

_TH_ Zheng(1993a) 0.72 4.28 -1.8 0 900 20

! Theoretical calculation by incremental method.

>> UVAROVITE/WATER GARNET #2 TEST <<------

_TH_ Zheng(1993a) 3.76 -9.05 2.52 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.85 -0.99 -2.03 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/UVAROVITE GARNET #3 TEST <<------

_TH_ Zheng(1993a) 0.26 4.39 -1.8 0 900 20

! Theoretical calculation by incremental method.

>> MELANITE/WATER GARNET #1 FIT <<------

_TH_ Richter&Hoernes(1988) 0.9 -0.98 -2.05 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation .

!!!! ---------- !!!!

!!!! ---------- EPIDOTES ---------- !!!!

>> ALLANITE/WATER PURE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 0.47 -1.13 -1.87 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/EPIDOTE EPIDOTE #1 FIT <<------

_TH_ Zheng(1993b) 0.42 3.05 -1.27 0 900 20

! Theoretical calculation by incremental method.

_NT_ Kohn&Valley(1998) 2.5 0 0 300 800 5

! No T range is given. T range from the references in the paper.

! 1sd on A coefficient = 0.15.

_MX_ Matthews(1994) 2.225 0 0 400 700 5

! Based on experimental data on Zo-water fractionation and on a correction based on the estimate of the effect of Fe3+ substitution by Kieffer(1982).

! Proposed A coeff = 2.00 + 0.75X, where X=mole fraction of pistacite (Ca2Fe3Si3O12OH) component in the epidote.Here X=0.30 is chosen.

_EX_ Matthews&Schliestedt(1984) 2.135 0 0 350 600 5

! Based on the experimental zo-water and qtz-water calibrations of Matthews&al(1983b) and Matsuhisa et al.(1979).

! Effect of Fe3+ substitution is estimated using the grossular/andradite data of Taylor(1976).

! Proposed A coeff = -1.56 -1.92X, where X=mole fractionation of pistacite (Ca2Fe3Si3O12OH) component in the epidote. Here X=0.30 is chosen.

>> EPIDOTE/WATER EPIDOTE #2 TEST <<------

_TH_ Zheng(1993b) 4.05 -7.81 2.29 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.85 -0.99 -2.03 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! No significant shift caused by Fe or Mn substitutions.

! Significant shift due to incorporation od Fe2+ in octahedral position and REE incorporation (i.e. allanite).

>> CALCITE/EPIDOTE EPIDOTE #3 TEST <<------

_TH_ Zheng(1993b) -0.04 3.15 -1.27 0 900 20

! Theoretical calculation by incremental method.

>> PIEMONTITE/WATER EPIDOTE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 0.85 -0.99 -2.03 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> ZOISITE/WATER EPIDOTE #1 FIT <<------

_TH_ Zheng(1993b) 4.05 -7.84 2.3 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.79 -1.02 -2.01 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! No significant shift caused by Fe or Mn substitutions.

! Significant shift due to incorporation of Fe2+ in octahedral position and REE incorporation (i.e. allanite).

_EX_ Matthews&al(1983c) 5.22 -10.63 4.80 400 700 5
**** 700 -0.62 0.07
**** 600 -0.50 0.05
**** 500 -0.33 0.01
**** 450 0.20 0.15
**** 400 0.49 0.14
! Parameters recalculated from the esperimental data. Uncertainties are 1sd of the different measuremets at each T.

!_EX_ Matthews&al(1983c) 4.97 -6.99 0 400 700 5
! ! Equation given in Cole&al(1987).

!_EX_ Matthews&al(1983c) 0.72 0 -1.34 400 700 5
! ! Parameters as reported in Richter&Hoernes(1988).

>> QUARTZ/ZOISITE EPIDOTE #2 TEST <<------

_TH_ Zheng(1993b) 0.43 3.07 1.28 0 900 20
! Theoretical calculation by incremental method.

_EX_ Matthews(1994) 2.00 0 0 400 700 5
! Quartz-water data from Chiba et al (1989)
! A pevious calibration by Matthews&al(1983b) resulted in A = 1.56.

>> CALCITE/ZOISITE EPIDOTE #3 TEST <<------

_TH_ Zheng(1993b) 0.04 3.18 -1.28 0 900 20
! Theoretical calculation by incremental method.

_EX_ Matthews(1994) 1.62 0 0 400 700 5
! Combining min-water data with quartz-water data from Matsuhisa&al(1979).
! A pevious calibration by Matthews&al(1983b) resulted in A = 1.06.

!!!! ---------- !!!!

!!!! ---------- AMPHIBOLES ---------- !!!!

>> QUARTZ/ACTINOLITE AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 0.52 3.48 -1.45 0 900 20
! Theoretical calculation by incremental method.

>> ACTINOLITE/WATER AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 3.96 -8.25 2.37 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/ACTINOLITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.05 3.58 -1.45 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/ANTHOPHYLLITE AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 0.52 3.49 -1.46 0 900 20

! Theoretical calculation by incremental method.

>> ANTHOPHYLLITE/WATER AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 3.96 -8.26 2.38 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/ANTHOPHYLLITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.06 3.6 -1.46 0 900 20

! Theoretical calculation by incremental method.

>> CUMMINGTONITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 3.96 -8.25 2.37 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.22 -0.86 -2.19 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/CUMMINGTONITE AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 0.52 3.48 -1.45 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/CUMMINGTONITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.05 3.58 -1.45 0 900 20

! Theoretical calculation by incremental method.

>> EDENITE/WATER		AMPHIBOLE			#1	FIT		<<------
_TH_	Richter&Hoernes(1988)	0.91	-0.97	-2.06	300	800	20	

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/EDENITE		AMPHIBOLE			#2	TEST		<<------
_TH_	Hoffbauer&al(1994)	2.61	0.00	0.00	600	900	20	

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> GEDRITE/WATER		AMPHIBOLE			#1	FIT		<<------
_TH_	Zheng(1993b)	3.85	-8.72	2.46	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Richter&Hoernes(1988)	1.03	-0.93	-2.11	300	800	20	

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/GEDRITE		AMPHIBOLE			#2	TEST		<<------
_TH_	Zheng(1993b)	0.63	3.96	-1.66	0	900	20	

! Theoretical calculation by incremental method.

>> CALCITE/GEDRITE		AMPHIBOLE			#3	TEST		<<------
_TH_	Zheng(1993b)	0.17	4.06	-1.66	0	900	20	

! Theoretical calculation by incremental method.

>> QUARTZ/GLAUCOPHANE		AMPHIBOLE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.45	3.18	-1.32	0	900	20	

! Theoretical calculation by incremental method.

_NT_	Kohn&Valley(1998c)	2.2	0	0	300	800	5	

! Based on literature data. No T range is given in the papaer. T range from the references in the papaer.

! 1sd on A coefficient = 0.25.

_MX_	Javoy&al(1970)	1.53	0	1.37	300	800	5	

! No T range is given, Here a reference T range for the stability field of Gln was chosen.

! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.

! Changed from the original papaer (symmetric fit with respect to x axis).

>> GLAUCOPHANE/WATER AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 4.03 -7.94 2.31 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.62 -0.73 -2.35 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/GLAUCOPHANE AMPHIBOLE #3 TEST <<------

_TH_ Hoffbauer&al(1994) 1.87 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> GRUNERITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 3.98 -8.17 2.36 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/GRUNERITE AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 0.50 3.40 -1.42 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/GRUNERITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.03 3.50 -1.42 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/HORNBLENDE AMPHIBOLE #2 FIT <<------

_TH_ Zheng(1993b) 0.59 3.80 -1.59 0 900 20

! Theoretical calculation by incremental method.

_MX_ Javoy&al(1970) 2.00 0.00 1.19 200 900 5

! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.

! Changed from the original papaer (symmetric fit with respect to x axis).

>> HORNBLENDE/WATER AMPHIBOLE #1 TEST <<------

_TH_ Zheng(1993b) 3.89 -8.56 2.43 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.12 -0.90 -2.14 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Parameters for Al-Mg-Hbl.

>> CALCITE/HORNBLENDE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.13 3.90 -1.59 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.40 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> KATOPHORITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 1.12 -0.9 -2.14 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/PARGASITE AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 0.71 4.22 -1.77 0 900 20

! Theoretical calculation by incremental method.

>> PARGASITE/WATER AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 3.77 -8.99 2.51 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.81 -1.01 -2.02 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/PARGASITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.24 4.32 -1.77 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.73 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> RICHTERITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 1.22 -0.87 -2.18 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> RIEBECKITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 4.05 -7.85 2.30 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/RIEBECKITE AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 0.43 3.08 -1.28 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/RIEBECKITE AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) -0.04 3.18 -1.28 0 900 20

! Theoretical calculation by incremental method.

>> TARAMITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 1.02 -0.94 -2.10 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> TREMOLITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Zheng(1993b) 3.95 -8.28 2.38 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.2 -0.87 -2.18 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/TREMOLITE AMPHIBOLE #2 TEST <<------

_TH_ Zheng(1993b) 0.53 3.52 -1.47 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/TREMOLITE AMPHIBOLE #3 TEST <<------

_TH_ Zheng(1993b) 0.06 3.62 -1.47 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.27 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> TSCHERMAKITE/WATER AMPHIBOLE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 1.02 -0.93 -2.1 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/TSCHERMAKITE AMPHIBOLE #2 TEST <<------

_TH_ Hoffbauer&al(1994) 2.53 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- CHLORITE ---------- !!!!

>> QUARTZ/CHAMOSITE CHLORITE #1 FIT <<------

_TH_ Zheng(1993b) 0.42 3.04 -1.27 0 900 20

! Theoretical calculation by incremental method.

>> CHAMOSITE/WATER CHLORITE #2 TEST <<------

_TH_ Zheng(1993b) 4.06 -7.81 2.3 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/CHAMOSITE CHLORITE #3 TEST <<------

_TH_ Zheng(1993b) -0.04 3.14 -1.27 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/CLINOCHLORE CHLORITE #1 FIT <<------

_TH_ Zheng(1993b) 0.51 3.43 -1.43 0 900 20

! Theoretical calculation by incremental method.

>> CLINOCHLORE/WATER CHLORITE #2 TEST <<------

_TH_ Zheng(1993b) 3.97 -8.19 2.36 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/CLINOCHLORE CHLORITE #3 TEST <<------

_TH_ Zheng(1993b) 0.04 3.53 -1.43 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/CHLORITE CHLORITE #1 FIT <<------

_NT_ Lacroix&Vennmann(2015) 1.63 0 2 240 550 5

! Based on natural samples. One of the most recent calibrations available.

>> CHLORITE/WATER CHLORITE #2 TEST <<------

_NT_ Wenner&Taylor(1971) 1.56 0 -4.7 150 400 5

! As reported in Chacko&al.(2001).

_TH_ Richter&Hoernes(1988) 0.81 -1.01 -2.01 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> THURINGITE/WATER CHLORITE #1 FIT <<------

_TH_ Zheng(1993b) 3.90 -8.50 2.42 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/THURINGITE CHLORITE #2 TEST <<------

_TH_ Zheng(1993b) 0.58 3.73 -1.56 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/THURINGITE CHLORITE #3 TEST <<------

_TH_ Zheng(1993b) 0.11 3.84 -1.56 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- WHITE MICAS ---------- !!!!

>> QUARTZ/MARGARITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.38 2.84 -1.18 0 900 20

! Theoretical calculation by incremental method.

>> MARGARITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 4.1 -7.61 2.25 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.87 -0.99 -2.04 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/MARGARITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.08 2.94 -1.18 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.76 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> QUARTZ/MUSCOVITE WHITEMICA #2 FIT <<------

_TH_ Zheng(1993b) 0.38 2.84 -1.18 0 900 20

! Theoretical calculation by incremental method.

_MX_ Matthews&Schliestedt(1984) 1.55 0.00 0.00 500 650 5

! Based on the experimental calibrations of O'Neil&Taylor(1969) and Matsuhisa et al.(1979); straight line constrained to the origin.

_MX_ Bottinga&Javoy(1973) 2.2 0.00 -0.6 500 800 5

! Based on the experimental data of O'Neil&Taylor(1969),natural samples, and theoretical estimate of the effect of OH groups on fractionation behavior.

_EX_ Chacko&al(1996) 1.39 0.00 -0.06 500 800 5

_EX_ Chacko&al(2001) 1.37 0.00 0.00 550 800 5

! Recalculated from experimental data of Chacko&al(1996)

_NT_ Kohn&Valley(1998a) 1.70 0.00 0.00 300 800 5

! Fractionations determined empirically. T range from the references in the paper.

! 1sd on A coefficient = 0.221.

_MX_ Javoy&al(1970) 1.22 0.00 1.11 400 800 5

! No T range is given, Here a reference T range for the stability field of Ms was chosen on the base of the other available T ranges.

! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.

! Changed from the original papaer (symmetric fit with respect to x axis).

>> MUSCOVITE/WATER WHITEMICA #1 TEST <<------

_TH_ Zheng(1993b) 4.10 -7.61 2.25 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.46 -0.78 -2.28 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Substitution of OH-groups by other anians (like F) causes a significant shift in the fractionation.

_EX_ O'Neil&Taylor(1969) 2.38 0.00 -3.89 400 650 5

**** 650 -1.26 0.20

**** 630 -0.94 0.20

**** 600 -0.82 0.20

**** 600 -0.78 0.20

**** 550 -0.30 0.20

**** 510 0.02 0.21

**** 500 -0.08 0.27

**** 420 1.01 0.22

**** 400 1.29 0.23

! Parameters obtained for both Pg and Mu micas. Experimental data reported here are for Kln and Ms gel.

! Data excluded by the athors are excluded.

! Analytical procedure maximum error(0.20, 1sd); SD of different measurements at the same T is propagated when available.

! Pramaters in agreement with the correction by Friedman&O'Neil(1977).

_MX_ Bottinga&Javoy(1973) 1.90 0.00 -3.10 500 800 5

! Based on the experimental data of O'Neil&Taylor(1969),natural samples, and theoretical estimate of the effect of OH groups on fractionation behavior.

! Pramaters in agreement with the correction by Friedman&O'Neil(1977).

>> CALCITE/MUSCOVITE WHITEMICA #3 TEST <<------

_TH_ Zheng(1993b) -0.08 2.97 -1.18 0 900 20

! Theoretical calculation by incremental method.

_EX_ Chacko&al(1996) 0.98 0.00 0.01 550 650 5

**** 650 1.15 0.25

**** 550 1.53 0.25

**** 500 1.91 0.25

**** 450 2.59 0.25

! Uncertainties in fractionation factors are not reported for each measurement, but they are ranging between 0.25 and 0.07. Here the maximum value is chosen.

! The coefficients represent an approximation of a more precise 3rd grade polynomial function valid at T>500°C.

_TH_ Hoffbauer&al(1994) 2.10 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

! The authors recognizd a mismatch with the data from natural samples.

>> PARAGONITE/WATER WHITEMICA #1 FIT <<------

_TH_ Zheng(1993b) 4.11 -7.54 2.24 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.37 -0.81 -2.25 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Substitution of OH-groups by other anians (like F) causes a significant shift in the fractionation.

_EX_ O'Neil&Taylor(1969) 2.38 0.00 -3.89 350 650 5

**** 600 -0.79 0.20

**** 550 0.18 0.20

**** 500 0.29 0.20

**** 420 1.03 0.20

**** 400 0.41 0.20

! Parameters obtained for both Pg and Mu micas. Experimental data reported here are only for Pg; data excluded by the athors are excluded.

! Error: analytical procedure maximum error as reported in the paper.

>> QUARTZ/PARAGONITE WHITEMICA #2 TEST <<------

_TH_ Zheng(1993b) 0.37 2.77 -1.15 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/PARAGONITE WHITEMICA #3 TEST <<------

_TH_ Zheng(1993b) -0.10 2.87 -1.15 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.10 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> PHENGITE/WATER WHITEMICA #1 FIT <<------

_TH_ Zheng(1993b) 4.13 -7.41 2.22 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.56 -0.75 -2.32 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Substitution of OH-groups by other anians (like F) causes a significant shift in the fractionation.

>> QUARTZ/PHENGITE WHITEMICA #2 TEST <<------

_TH_ Zheng(1993b) 0.35 2.64 -1.10 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/PHENGITE WHITEMICA #3 TEST <<------

_TH_ Zheng(1993b) -0.12 2.74 -1.10 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 1.97 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- BIOTITE MICAS ---------- !!!!

>> QUARTZ/ANNITE BIOTITE #1 FIT <<------

_TH_ Zheng(1993b) 0.59 3.79 -1.59 0 900 20

! Theoretical calculation by incremental method.

>> ANNITE/WATER BIOTITE #2 TEST <<------

_TH_ Zheng(1993b) 3.89 -8.56 2.43 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.67 -1.06 -1.95 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/ANNITE BIOTITE #3 TEST <<------

_TH_ Zheng(1993b) 0.13 3.89 -1.59 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/BIOTITE BIOTITE #1 FIT <<------

_TH_ Zheng(1993b) 0.64 3.99 -1.67 0 900 20

! Theoretical calculation by incremental method.

_NT_ Bottinga&Javoy(1975) 3.69 0.00 -0.60 500 900 5

! No maximum reliable T is given. Minimum T = 500°C.

_MX_ Javoy&al(1970) 2.95 0.00 1.12 500 900 5

! No T range is given, Here a reference T range for the stability field of Bt was chosen.

! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.

! Changed from the original papaer (symmetric fit with respect to x axis).

>> BIOTITE/WATER		BIOTITE			#2	TEST		<<------
_TH_	Zheng(1993b)	3.84	-8.76	2.46	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Richter&Hoernes(1988)	0.66	-1.06	-1.95	300	800	20	
! Water parameters are taken from experimental data from the literature (not specified).								
! An "average qtz-water curve" forms the basis for the increment method calculation.								
! Substitution of OH-groups by other anians (like F) causes a significant shift in the fractionation.								
>> CALCITE/BIOTITE		BIOTITE			#3	TEST		<<------
_TH_	Zheng(1993b)	0.18	4.10	-1.67	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Hoffbauer&al(1994)	2.58	0.00	0.00	600	900	20	
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).								
! Parameters for Fe-Biotite with Fe3+.								
_TH_	Hoffbauer&al(1994)	2.90	0.00	0.00	600	900	20	
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).								
! Parameters for Mg-Biotite with Mg4Al1.67.								
_TH_	Hoffbauer&al(1994)	3.17	0.00	0.00	600	900	20	
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).								
! Parameters for Mg-Biotite with Mg6Al0.33.								
>> QUARTZ/F-PHLOGOPITE		BIOTITE			#1	FIT		<<------
_EX_	Chacko&al(2001)	1.64	0.00	0.00	500	800	5	
! Recalculated from experimental data of Chacko&al(1996).								
>> CALCITE/F-PHLOGOPITE		BIOTITE			#2	TEST		<<------
_EX_	Chacko&al(1996)	1.26	0.00	0.00	500	800	5	
! Experiments at 15 kbar.								
! F/(F+OH) = 1.								
_EX_	Fortier&al(1994)	1.84	0.00	0.43	400	800	5	
! Experiments at 11 kbar.								
! F/(F+OH) = 0.75.								
>> PHLOGOPITE/WATER		BIOTITE			#1	FIT		<<------
_TH_	Zheng(1993b)	3.86	-8.68	2.45	0	900	20	

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.65 -1.06 -1.95 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Substitution of OH-groups by other anians (like F) causes a significant shift in the fractionation.

>> QUARTZ/PHLOGOPITE BIOTITE #2 TEST <<------

_TH_ Zheng(1993b) 0.62 3.92 -1.64 0 900 20

! Theoretical calculation by incremental method.

_EX_ Chacko&al(2001) 2.16 0.00 0.00 500 800 5

! Recalculated from experimental data of Chacko&al(1996).

>> CALCITE/PHLOGOPITE BIOTITE #3 TEST <<------

_TH_ Zheng(1993b) 0.16 4.02 -1.64 0 900 20

! Theoretical calculation by incremental method.

_EX_ Chacko&al(1996) 1.78 0.00 0.00 650 800 5

**** 800 1.42 0.25

**** 700 1.81 0.25

**** 650 2.30 0.25

**** 650 2.03 0.25

! Uncertainties in fractionation factors for each measurement are not reported, but they range between 0.25 and 0.07. Here the maximum value is chosen.

! The coefficients represent an approximation of a more precise 3rd grade polynomial function.

_TH_ Hoffbauer&al(1994) 2.91 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- OTHER MICAS ---------- !!!!

>> QUARTZ/GLAUCONITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.49 3.34 -1.39 0 900 20

! Theoretical calculation by incremental method.

>> GLAUCONITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 3.99 -8.11 2.34 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.79 -0.97 -2.42 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/GLAUCONITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.02 3.44 -1.39 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/LEPIDOLITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.38 2.81 -1.17 0 900 20

! Theoretical calculation by incremental method.

>> LEPIDOLITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 4.10 -7.58 2.25 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.54 -0.76 -2.32 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/LEPIDOLITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.09 2.91 -1.17 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- CLINOPYROXENE ---------- !!!!

>> QUARTZ/ACMITE CLINOPYROXENE #1 FIT <<------

_TH_ Zheng(1993a) 0.30 2.38 -0.99 0 900 20

! Theoretical calculation by incremental method.

>> ACMITE/WATER CLINOPYROXENE #2 TEST <<------

_TH_ Zheng(1993a) 4.18 -7.14 2.17 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.13 -0.55 -2.56 300 800 20

! Reported as Aegirine

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/ACMITE CLINOPYROXENE #3 TEST <<------

_TH_ Zheng(1993a) -0.17 2.45 -0.99 0 900 20

! Theoretical calculation by incremental method.

!>> AEGIRINE/WATER CLINOPYROXENE #1 FIT <<------

!

!_TH_ Richter&Hoernes(1988) 2.13 -0.55 -2.56 300 800 20

! ! Water parameters are taken from experimental data from the literature (not specified).

! ! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/DIOPSIDE CLINOPYROXENE #1 FIT <<------

_TH_ Zheng(1993a) 0.56 3.67 -1.53 0 900 20

! Theoretical calculation by incremental method.

!_EX_ Chiba&al(1989) 2.75 0.00 0.00 600 1200 5

! ! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).

! ! Fractionation data combined with the data of Clayton&al(1989).

! ! Standard error of the coefficient = 0.10.

_EX_ Chiba&al(1989) 2.75 0.00 0.00 600 900 5

! Reduced T range.

_EX_ Matthews&al(1983a) 2.08 0.00 0.00 400 800 5

! Pyroxene-water fractionation was experimetally studied. Quartz and feldspar data from Matsuhisa&al(1979).

>> DIOPSIDE/WATER CLINOPYROXENE #2 TEST <<------

_TH_ Zheng(1993a) 3.92 -8.43 2.40 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.18 -0.88 -2.17 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Parameters valid when Si is the only tetrahedrally coordinated cation.

>> CALCITE/DIOPSIDE CLINOPYROXENE #3 TEST <<------

_TH_ Zheng(1993a) 0.10 3.78 -1.53 0 900 20

! Theoretical calculation by incremental method.

!_EX_	Chiba&al(1989)			2.37	0.00	0.00	600	1200	5
!****	600	3.17	0.14						
!****	700	2.45	0.14						
!****	800	2.09	0.14						
!****	1000	1.43	0.14						
!****	1200	1.01	0.14						

! ! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).

! ! Fractionation data combined with the data of Clayton&al(1989).

! ! Correlation coefficient = 0.997.

! ! Standard error of the coefficient = 0.07.

_EX_	Chiba&al(1989)	2.37	0.00	0.00	600	900	5	

! Reduced T range.

_TH_	Hoffbauer&al(1994)	2.30	0.00	0.00	600	900	20	

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> HEDENBERGITE/WATER		CLINOPYROXENE			#1	FIT		<<------
_TH_	Zheng(1993a)	3.93	-8.37	2.40	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Richter&Hoernes(1988)	1.19	-0.88	-2.17	300	800	20	

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Parameters valid when Si is the only tetrahedrally coordinated cation.

>> QUARTZ/HEDENBERGITE		CLINOPYROXENE			#2	TEST		<<------
_TH_	Zheng(1993a)	0.55	3.61	-1.51	0	900	20	

! Theoretical calculation by incremental method.

>> CALCITE/HEDENBERGITE		CLINOPYROXENE			#3	TEST		<<------
_TH_	Zheng(1993a)	0.08	3.71	-1.51	0	900	20	

! Theoretical calculation by incremental method.

>> QUARTZ/JADEITE		CLINOPYROXENE			#1	FIT		<<------
_TH_	Zheng(1993a)	0.31	2.42	-1.01	0	900	20	

! Theoretical calculation by incremental method.

_EX_	Matthews(1994)	1.69	0.00	0.00	400	600	5	

! Combining min-water data with quartz-water data from Matsuhisa&al(1979).

_EX_ Matthews&al(1983a) 1.09 0.00 0.00 400 800 5

! Pyroxene-water fractionation was experimetally studied. Quartz and feldspar data from Matsuhisa&al(1979).

>> JADEITE/WATER CLINOPYROXENE #2 TEST <<------

_TH_ Zheng(1993a) 4.17 -7.19 2.18 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.99 -0.60 -2.50 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Parameters valid when Si is the only tetrahedrally coordinated cation.

_EX_ Matthews(1994) 4.62 -10.19 5.82 400 600 5

**** 600 0.21 0.02

**** 500 0.37 0.02

**** 400 0.88 0.15

! Equation recalculated from the experimental points reported in tha paper (fractionation calibrated by Matthews&al(1983c)).

>> CALCITE/JADEITE CLINOPYROXENE #3 TEST <<------

_TH_ Zheng(1993a) -0.16 2.52 -1.01 0 900 20

! Theoretical calculation by incremental method.

_EX_ Matthews(1994) 1.31 0.00 0.00 400 600 5

! Combining min-water data with quartz-water data from Matsuhisa&al(1979).

_TH_ Hoffbauer&al(1994) 1.49 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- ORTHOPYROXENE ---------- !!!!

>> ENSTATITE/WATER ORTHOPYROXENE #1 FIT <<------

_TH_ Zheng(1993a) 3.97 -8.22 2.37 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.18 -0.88 -2.17 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

! Parameters valid when Si is the only tetrahedrally coordinated cation.

>> QUARTZ/ENSTATITE ORTHOPYROXENE #2 TEST <<------

_TH_ Zheng(1993a) 0.51 3.45 -1.44 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.52 0.88 -1.04 300 800 20
! Parameters reported in Kohn(1993).

>> CALCITE/ENSTATITE ORTHOPYROXENE #3 TEST <<------

_TH_ Zheng(1993a) 0.05 3.55 -1.44 0 900 20
! Theoretical calculation by incremental method.

>> FERROSILITE/WATER ORTHOPYROXENE #1 FIT <<------

_TH_ Zheng(1993a) 3.99 -8.09 2.35 0 900 20
! Theoretical calculation by incremental method.

>> QUARTZ/FERROSILITE ORTHOPYROXENE #2 TEST <<------

_TH_ Zheng(1993a) 0.48 3.33 -1.39 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.49 0.87 -1.03 300 800 20
! Parameters reported in Kohn(1993).

>> CALCITE/FERROSILITE ORTHOPYROXENE #3 TEST <<------

_TH_ Zheng(1993a) 0.02 3.43 -1.39 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- OLIVINE ---------- !!!!

>> FAYALITE/WATER OLIVINE #1 FIT <<------

_TH_ Zheng(1993a) 3.64 -9.46 2.59 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) -0.04 -1.31 -1.66 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/FAYALITE OLIVINE #2 TEST <<------

_TH_ Zheng(1993a) 0.84 4.69 -1.97 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 3.74 1.31 -1.55 300 800 20
! Parameters reported in Kohn(1993).

>> CALCITE/FAYALITE OLIVINE #3 TEST <<------

_TH_ Zheng(1993a) 0.38 4.79 -1.97 0 900 20
! Theoretical calculation by incremental method.

>> FORSTERITE/WATER OLIVINE #1 FIT <<------

_TH_ Zheng(1993a) 3.55 -9.72 2.64 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) -0.07 -1.32 -1.65 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/FORSTERITE OLIVINE #2 TEST <<------

_TH_ Zheng(1993a) 0.93 4.95 -2.09 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 3.77 1.32 -1.56 300 800 20
! Parameters reported in Kohn(1993).

!_EX_ Chiba&al(1989) 3.67 0 0 200 1200 5
! ! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).
! ! Fractionation data combined with the data of Clayton&al(1989).
! ! Standard error of the coefficient = 0.11.

_EX_ Chiba&al(1989) 3.67 0 0 200 900 5
! Reduced T range.

>> CALCITE/FORSTERITE OLIVINE #3 TEST <<------

_TH_ Zheng(1993a) 0.46 5.05 -2.09 0 900 20
! Theoretical calculation by incremental method.

_EX_ Zheng&al(1994) 3.17 0 0.44 600 900 5

_TH_ Hoffbauer&al(1994) 3.64 0 0 600 900 20

```
     ! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!_EX_       Chiba&al(1989)                  3.29    0       0           700     1200    5
!****       700     3.30    0.14
!****       800     2.97    0.14
!****       1000    1.93    0.14
!****       1000    2.18    0.14
!****       1200    1.44    0.14
!****       1300    1.54    0.14
!     ! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).
!     ! Fractionation data combined with the data of Clayton&al(1989).
!     ! Correlation coefficient = 0.978.
!     ! Standard error of the coefficient = 0.08.

_EX_        Chiba&al(1989)                  3.29    0       0           700     900     5
     ! Reduced T range.


>> QUARTZ/TEPHROITE                         OLIVINE                     #1      FIT             <<------

_TH_        Zheng(1993a)                    0.86    4.75    -2.0        0       900     20
     ! Theoretical calculation by incremental method.


>> TEPHROITE/WATER                  OLIVINE                        #2      TEST            <<------

_TH_        Zheng(1993a)                    3.62    -9.51   2.6         0       900     20
     ! Theoretical calculation by incremental method.


>> CALCITE/TEPHROITE                        OLIVINE                     #3      TEST            <<------

_TH_        Zheng(1993a)                    0.39    4.85    -2.0        0       900     20
     ! Theoretical calculation by incremental method.



!!!! ------------------------------------------------------------------------------------------------------------ !!!!

!!!! ------------------------------------------------------ ZEOLITES ------------------------------------------------ !!!!


>> ANALCIME/WATER                           PURE                        #1      FIT             <<------

_MX_        Karlsson&Clayton(1990)          2.78    0.00    -2.89       25      400     5
****        400     2.90    0.4
****        350     4.50    0.4
****        300     5.80    0.4
****        145     12.20   0.2
****        55      24.2    0.2
```

**** 30 28.2 0.2

! Values at 300, 350 and 400 C from experiments; other values from natural samples.

! Direct exchange. P = 1.5 - 5.0 kbar.

>> STILBITE/WATER PURE #1 FIT <<------

_EX_ Feng&Savin(1993) 2.70 0.00 -2.40 220 300 5

! Direct exchange at very low pressure (21 Torr).

>> WAIRAKITE/WATER PURE #1 FIT <<------

_EX_ Noto&Kusakabe(1997) 0.79 0.00 -3.07 250 400 5

**** 400 -1.55 0.11

**** 350 -0.87 0.13

**** 350 -0.94 0.11

**** 330 -0.69 0.09

**** 300 -0.77 0.36

**** 270 -0.71 0.46

**** 270 -0.21 0.69

**** 250 -0.11 0.08

! Direct exchange at 0.5-1.5 kbar.

! Here the equation calculated from 94-99% exchange experiments is selected.

! Parameters obtained from 63-98% exchange experiments: A=2.46, B=0.00, C=-1.76.

!!!! ---------- !!!!

!!!! ---------- Al-SILICATES ---------- !!!!

>> QUARTZ/ANDALUSITE PURE #1 FIT <<------

_TH_ Zheng(1993c) 0.28 2.26 -0.94 0 900 20

! Theoretical calculation by incremental method.

!_NT_ Sharp(1995) 2.25 0 0 535 1300 5

! ! Fractionation of aluminosilicates is considered to be the same 2.25 +-0.2.

! ! Assumptions: Fractionation(qtz-grt) known; qtz,grt,Al2SiO5 in equilibrium.

! ! T estimates from oxygen isotope thermometry are calibrated to the T coeff for qtz-grt.

_NT_ Sharp(1995) 2.25 0 0 535 900 5

! Reduced T range.

>> ANDALUSITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993c) 4.2 -7.02 2.15 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.96 -0.61 -2.49 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/ANDALUSITE PURE #3 TEST <<------

_TH_ Zheng(1993c) -0.19 2.36 -0.94 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.25 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> QUARTZ/KYANITE PURE #1 FIT <<------

_TH_ Zheng(1993c) 0.32 2.52 -1.05 0 900 20

! Theoretical calculation by incremental method

!_NT_ Sharp(1995) 2.17 0 0 535 1300 5

! ! Fractionations of aluminosilicates is considered to be the same at 2.25 +-0.2.

! ! Assumptions: Fractionation(qtz-grt) known; qtz,grt,Al2SiO5 in equilibrium.

! ! T estimates from oxygen isotope thermometry are calibrated to the T coeff for qtz-grt.

_NT_ Sharp(1995) 2.17 0 0 535 900 5

! Reduced T range.

>> KYANITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993c) 4.16 -7.29 2.2 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.72 -0.69 -2.39 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/KYANITE PURE #3 TEST <<------

_TH_ Zheng(1993c) -0.14 2.63 -1.05 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.49 0 0 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

_EX_ Tennie&al(1998) 2.62 0 0 625 775 5

**** 625 3.12 0.23

**** 675 3.16 0.14
**** 725 2.60 0.11
**** 775 2.30 0.55
! Kyanite-Calcium carbonate exchange experiments.
! Uncertainty on A +-0.2 calculated as deviation of the individual experimental runs from the calculated equilibrium.
! 1SD on the experimental points calculated as SD of experimental runs at the same T.

>> QUARTZ/SILLIMANITE PURE #1 FIT <<------

_TH_ Zheng(1993c) 0.22 1.89 -0.78 0 900 20
! Theoretical calculation by incremental method.

!_NT_ Sharp(1995) 2.36 0.00 0.00 535 1300 5
! ! Fractionations of aluminosilicates is considered to be the same 2.25 +-0.2.
! ! Assumptions: Fractionation(qtz-grt) known; qtz,grt,Al2SiO5 in equilibrium.
! ! T estimates from oxygen isotope thermometry are calibrated to the T coeff for qtz-grt.

_NT_ Sharp(1995) 2.36 0.00 0 .00 535 900 5
! Reduced T range.

>> SILLIMANITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993c) 4.26 -6.65 2.07 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 2.3 -0.48 -2.64 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/SILLIMANITE PURE #3 TEST <<------

_TH_ Zheng(1993c) -0.25 1.99 -0.78 0 900 20
! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 1.84 0.00 0.00 600 900 20
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> QUARTZ/TOPAZ PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.30 2.41 -1.00 0 900 20
! Theoretical calculation by incremental method.

>> TOPAZ/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 4.18 -7.18 2.17 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/TOPAZ PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.16 2.52 -1.00 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- CHLORITOID ---------- !!!!

>> QUARTZ/CHLORITOID PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.49 3.35 -1.40 0 900 20
! Theoretical calculation by incremental method.

>> CHLORITOID/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 3.99 -8.11 2.35 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/CHLORITOID PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.02 3.45 -1.40 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- SPINEL ---------- !!!!

>> QUARTZ/HERCYNITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.92 9.80 -5.24 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.37 7.87 -3.39 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> HERCYNITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.32 -13.58 4.20 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.11 -12.63 3.05 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/HERCYNITE		PURE			#3	TEST		<<------
_TH_	Zheng(1991)	1.90	7.97	-3.39	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								
>> QUARTZ/SPINEL		SPINEL			#1	FIT		<<------
!_TH_	Zheng(1991)	2.06	10.04	-5.38	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Zheng(1991)	2.51	8.06	-3.48	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								
>> SPINEL/WATER		SPINEL			#2	TEST		<<------
!_TH_	Zheng(1991)	2.18	-13.81	4.34	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Zheng(1991)	1.97	-12.82	3.07	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								
>> CALCITE/SPINEL		SPINEL			#3	TEST		<<------
_TH_	Zheng(1991)	2.05	8.16	-3.48	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								
>> QUARTZ/ULVOESPINEL		PURE			#1	FIT		<<------
!_TH_	Zheng(1991)	1.43	8.78	-4.67	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Zheng(1991)	1.84	7.04	-3.01	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								
>> ULVOESPINEL/WATER		PURE			#2	TEST		<<------
!_TH_	Zheng(1991)	2.81	-12.56	3.63	0	900	20	
! Theoretical calculation by incremental method.								
_TH_	Zheng(1991)	2.64	-11.81	2.95	0	900	20	
! Theoretical calculation by incremental method (revised, Table 2).								

>> CALCITE/ULVOESPINEL PURE #3 TEST <<------

_TH_ Zheng(1991) 1.37 7.15 -3.01 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

!!!! ---------- !!!!

!!!! ---------- ILMENITE ---------- !!!!

>> QUARTZ/GEIKELITE ILMENITE #1 FIT <<------

!_TH_ Zheng(1991) 1.46 8.85 -4.70 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.87 7.10 -3.04 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> GEIKELITE/WATER ILMENITE #2 TEST <<------

!_TH_ Zheng(1991) 2.78 -12.63 3.66 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.61 -11.86 2.96 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/GEIKELITE ILMENITE #3 TEST <<------

_TH_ Zheng(1991) 1.40 7.20 -3.04 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/ILMENITE ILMENITE #1 FIT <<------

!_TH_ Zheng(1991) 1.36 8.61 -4.57 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.76 6.90 -2.95 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> ILMENITE/WATER ILMENITE #2 TEST <<------

!_TH_ Zheng(1991) 2.88 -12.38 3.53 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.72 -11.67 2.94 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/ILMENITE ILMENITE #3 TEST <<------

_TH_ Zheng(1991) 1.29 7.01 -2.95 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

!!!! ---------- !!!!

!!!! ---------- STAUROLITE ---------- !!!!

>> STAUROLITE/WATER STAUROLITE #1 FIT <<------

_TH_ Zheng(1993b) 4.09 -7.66 2.27 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.83 -1.00 -2.02 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/STAUROLITE STAUROLITE #2 TEST <<------

_TH_ Zheng(1993b) 0.39 2.90 -1.21 0 900 20

! Theoretical calculation by incremental method.

_NT_ Kohn&Valley(1998a) 2.4 0.00 0.00 525 575 5

! Fractionations determined empirically. T range from the references in the paper.

>> CALCITE/STAUROLITE STAUROLITE #3 TEST <<------

_TH_ Zheng(1993b) -0.07 3.00 -1.21 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.80 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- CORDIERITE ---------- !!!!

>> QUARTZ/CORDIERITE PURE #1 FIT <<------

_TH_ Zheng(1993a) 0.38 2.85 -1.19 0 900 20
! Theoretical calculation by incremental method.

>> CORDIERITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 4.10 -7.62 2.26 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/CORDIERITE PURE #3 TEST <<------

_TH_ Zheng(1993a) -0.08 2.95 -1.19 0 900 20
! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 0.62 0.00 0.00 600 900 20
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- SALT ---------- !!!!

>> QUARTZ/PORTLANDITE PURE #1 FIT <<------

_TH_ Zheng(1998) 1.23 5.79 -2.45 0 900 20
! Theoretical calculation by incremental method.

>> PORTLANDITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1998) 3.25 -10.56 2.77 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/PORTLANDITE PURE #3 TEST <<------

_TH_ Zheng(1998) 0.77 5.89 -2.45 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- PHOSPHATES ---------- !!!!

>> CALCITE/APATITE PURE #1 FIT <<------

!_TH_ Zheng(2016) 0.68 1.15 -0.52 0 900 20

! ! Theoretical calculation by incremental method.Data for OH-apatite.

_EX_ Fortier&Lüttge(1995) 1.6 0.00 0.68 500 800 10

! P = 1.1 kbar.

! The curve is not valid below 500 °C.

! Experimental technique of Clayton&al(1989). NaCl confining material.

! Strongly discordant with the other data for apatite.

_EX_ Chacko&al(2001) 2.13 0.00 0.00 500 800 5

! Following Chacko&al.(1996), Fortier&Lüttge's 500-800°C apatite-calcite fractionation data have been regressed by a straight line through the origin.

>> QUARTZ/APATITE PURE #2 TEST <<------

!_TH_ Zheng(2016) 1.15 1.05 -0.52 0 900 20

! ! Theoretical calculation by incremental method.

_EX_ Chacko&al(2001) 2.51 0.00 0.00 500 800 5

! Following Chacko&al(1996), Fortier&Lüttge's 500-800°C apatite-calcite fractionation data have been regressed by a straight line through the origin.

!>> ClAPATITE/WATER PURE #1 FIT <<------

!_TH_ Zheng(1996) 3.75 -7.02 2.15 0 900 20

! ! Theoretical calculation by incremental method.

!_TH_ Zheng(2016) 3.52 -5.49 0.32 0 900 20

! ! Theoretical calculation by incremental method.

!>> QUARTZ/ClAPATITE PURE #2 TEST <<------

!_TH_ Zheng(1996) 0.73 2.25 -0.97 0 900 20

! ! Theoretical calculation by incremental method.

!_TH_ Zheng(2016) 0.96 0.73 -0.38 0 900 20

! ! Theoretical calculation by incremental method.

!>> CALCITE/ClAPATITE PURE #3 TEST <<------

!_TH_ Zheng(1996) 0.27 2.35 -0.97 0 900 20

! ! Theoretical calculation by incremental method.

!_TH_ Zheng(2016) 0.49 0.83 -0.38 0 900 20

! ! Theoretical calculation by incremental method.

!>> FAPATITE/WATER		PURE			#1	FIT		<<------
!_TH_	Zheng(1996)	3.81	-6.63	2.08	0	900	20	
!	! Theoretical calculation by incremental method.							
!_TH_	Zheng(2016)	3.53	-5.48	0.31	0	900	20	
!	! Theoretical calculation by incremental method.							
!>> QUARTZ/FAPATITE		PURE			#2	TEST		<<------
!_TH_	Zheng(1996)	0.67	1.87	-0.81	0	900	20	
!	! Theoretical calculation by incremental method.							
!_TH_	Zheng(2016)	0.95	0.71	-0.37	0	900	20	
!	! Theoretical calculation by incremental method.							
!>> CALCITE/FAPATITE		PURE			#3	TEST		<<------
!_TH_	Zheng(1996)	0.21	1.97	-0.81	0	900	20	
!	! Theoretical calculation by incremental method.							
!_TH_	Zheng(2016)	0.48	0.81	-0.37	0	900	20	
!	! Theoretical calculation by incremental method.							
!>> HYDROXIAPATITE/WATER		PURE			#1	FIT		<<------
!_TH_	Zheng(1996)	3.83	-6.48	2.05	0	900	20	
!	! Theoretical calculation by incremental method.							
!_TH_	Zheng(2016)	3.33	-5.81	0.46	0	900	20	
!	! Theoretical calculation by incremental method.							
!>> QUARTZ/HYDROXIAPATITE		PURE			#2	TEST		<<------
!_TH_	Zheng(1996)	0.65	1.71	-0.75	0	900	20	
!	! Theoretical calculation by incremental method.							
!_TH_	Zheng(2016)	1.15	1.05	-0.52	0	900	20	
!	! Theoretical calculation by incremental method.							
!>> CALCITE/HYDROXIAPATITE		PURE			#3	TEST		<<------
!_TH_	Zheng(1996)	0.19	1.81	-0.75	0	900	20	
!	! Theoretical calculation by incremental method.							

!_TH_ Zheng(2016) 0.68 1.15 -0.52 0 900 20

! ! Theoretical calculation by incremental method.

!>> MONAZITE/WATER PURE #1 FIT <<------

!

!_TH_ Zheng(1996) 4.22 -4.58 1.72 0 900 20

! ! Theoretical calculation by incremental method.

>> QUARTZ/MONAZITE PURE #1 FIT <<-----

!_TH_ Zheng(1996) 0.26 -0.18 0.05 0 1200 10

! ! Theoretical calculation by incremental method.

_TH_ Rubatto&al.(2014) 1.05 0.89 -0.45 0 900 20

! Data for Ce-Monazite.

!_MX_ Breecker&Sharp(2007) 2.20 0.00 0.00 390 1000 5

! ! Natural data + piston cylinder experiments.

! ! Monazites considered have intermediate compositions (not pure end-members)

_MX_ Breecker&Sharp(2007) 2.20 0.00 0.00 390 900 5

! Reduced T range.

!>> CALCITE/MONAZITE PURE #3 TEST <<------

!

!_TH_ Zheng(1996) -0.20 -0.08 0.05 0 900 20

! ! Theoretical calculation by incremental method.

>> XENOTIME/WATER PURE #1 FIT <<------

_TH_ Zheng(1996) 4.60 -4.45 1.75 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/XENOTIME PURE #2 TEST <<------

_TH_ Zheng(1996) -0.13 -0.32 0.14 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/XENOTIME PURE #3 TEST <<------

_TH_ Zheng(1996) -0.59 -0.22 0.14 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- HUMITES ---------- !!!!

>> CHONDRODITE/WATER		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	3.73	-9.11	2.52	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/CHONDRODITE		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	0.74	4.34	-1.82	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/CHONDRODITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	0.27	4.45	-1.82	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/CLINOHUMITE		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.70	4.19	-1.75	0	900	20	
! Theoretical calculation by incremental method.								
>> CLINOHUMITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	3.78	-8.95	2.50	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/CLINOHUMITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	0.23	4.29	-1.75	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/HUMITE		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.71	4.24	-1.78	0	900	20	
! Theoretical calculation by incremental method.								
>> HUMITE/WATER		PURE			#2	TEST		<<------

_TH_ Zheng(1993b) 3.77 -9.01 2.51 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/HUMITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.24 4.34 -1.78 0 900 20
! Theoretical calculation by incremental method.

>> NORBERGITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 3.62 -9.51 2.60 0 900 20
! Theoretical calculation by incremental method.

>> QUARTZ/NORBERGITE PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.86 4.75 -2.00 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/NORBERGITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.39 4.85 -2.00 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- HYDROXIDES ---------- !!!!

>> AKAGANEITE/WATER PURE #1 FIT <<------

_EX_ Bao&Koch(1999) 3.93 0.00 -12.16 35 95 5
! Synthetsis of akaganeite by hydrolysis of FeCl3 solutions.

>> BRUCITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1998) 3.23 -10.60 2.78 0 900 20
! Theoretical calculation by incremental method.

_EX_ Saccocia&al(1998) 9.54 -35.30 26.58 250 450 10
**** 250 -6.0 1.3
**** 350 -5.5 0.7
**** 450 -3.9 0.2

**** 350 -5.5 0.6

! P = 0.5 kbar.

! 3% and 10% NaCl solution. The results of the experiments are recalculated for pure water.

_EX_ Xu&Zheng(1999) 1.56 0.00 -14.1 15 120 10

**** 15 4.78 0.20

**** 25 3.89 0.10

**** 40 2.10 0.20

**** 50 1.10 0.10

**** 70 -0.60 0.20

**** 90 -2.10 0.30

**** 105 -3.21 0.00

**** 120 -3.31 0.10

! SD are from different experiments at the same T.

! Precipitation of brucite in aqueous solutions from MgCl2, Mg3N2 or MgO.

!_TH_ Savin&Lee(1988) -2.49 21.70 -34.76 0 800 20

! ! The authors considered the oxygen in brucite to be bonded entirely as M-OH bonds and estimated the fractionation on the bond-type approach.

! ! Equation fitted to data from metamorphic biotite-muscovite assemblages at HT and estimations at LT from a combination of the goethite-water.

! ! Data of Yapp(1987) with the M-O-M curve of Savin&Lee(1988).

! ! Clear disagreement with all the other calibrations available in the literature.

>> QUARTZ/BRUCITE PURE #2 TEST <<------

_TH_ Zheng(1998) 1.25 5.83 -2.47 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/BRUCITE PURE #2 TEST <<------

_TH_ Zheng(1998) 0.78 5.93 -2.47 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/DIASPORE PURE #1 FIT <<------

_TH_ Zheng(1998) 1.38 6.13 -2.60 0 900 20

! Theoretical calculation by incremental method.

>> DIASPORE/WATER PURE #2 TEST <<------

_TH_ Zheng(1998) 3.10 -10.89 2.82 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/DIASPORE PURE #3 TEST <<------

_TH_ Zheng(1998) 0.91 6.23 -2.60 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/BOEHMITE			PURE			#1	FIT	<<------
_TH_	Zheng(1998)		1.36	6.10	-2.59	0	900	20

! Theoretical calculation by incremental method.

>> BOEHMITE/WATER			PURE			#2	TEST	<<------
_TH_	Zheng(1998)		3.11	-10.87	2.81	0	900	20

! Theoretical calculation by incremental method.

>> CALCITE/BOEHMITE			PURE			#3	TEST	<<------
_TH_	Zheng(1998)		0.90	6.20	-2.59	0	900	20

! Theoretical calculation by incremental method.

>> QUARTZ/GEOTHITE			PURE			#1	FIT	<<------
_TH_	Zheng(1998)		1.17	5.62	-2.38	0	900	20

! Theoretical calculation by incremental method.

>> GEOTHITE/WATER			PURE			#2	TEST	<<------
_TH_	Zheng(1998)		3.31	-10.39	2.74	0	900	20

! Theoretical calculation by incremental method.

_EX_	Yapp(1987)		1.66	0.00	-12.7	0	70	5

! Different experimental methods. Only the results suggesting that the equilibrium values have been attained, or closely approached, were considered by the author.

_EX_	Yapp(1990)		1.63	0.00	-12.3	25	120	5
****	25	6.18	0.17					
****	44	3.49	0.14					
****	62	2.15	0.07					

! Yapp(1991) suggested that goethite does not exchange oxygen isotopes with the environment in the absence of dissolution and reprecipitation.

! Exp. points are reported with 1SD on all the measurements at the same temperature.

_EX_	Bao&Koch(1999)	1.91	0.00	-8.00	35	140	5

! Synthetsis of akaganeite by hydrolysis of FeCl3 solutions by addition of NaOH solution.

_EX_	Müller(1995)	1.10	0.00	-12.10	10	65	5

! Precipitation of Fe(NO3)2 solution by titrating KOH solution.

_EX_	Müller(1995)	0.30	0.00	-3.00	10	65	5

! Precipitation of Fe(NO3)2 solution by titrating NaOH solution.

_EX_ Müller(1995) 2.76 0.00 -23.7 10 65 5

! Precipitation of Fe(NO3)2 solution by hydrolysis.

>> CALCITE/GEOTHITE PURE #3 TEST <<------

_TH_ Zheng(1998) 0.70 5.73 -2.38 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/LEPIDOCROCITE PURE #1 FIT <<------

_TH_ Zheng(1998) 1.16 5.60 -2.37 0 900 20

! Theoretical calculation by incremental method.

>> LEPIDOCROCITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1998) 3.32 -10.37 2.74 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/LEPIDOCROCITE PURE #3 TEST <<------

_TH_ Zheng(1998) 0.69 5.70 -2.37 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/GIBBSITE PURE #1 FIT <<------

_TH_ Zheng(1998) 0.58 3.76 -1.57 0 900 20

! Theoretical calculation by incremental method.

>> GIBBSITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1998) 3.89 -8.52 2.42 0 900 20

! Theoretical calculation by incremental method.

_EX_ Bird&al(1994) 1.31 0.00 -0.78 8 51 5

**** 8 16.07 1.18

**** 22 13.80 0.30

**** 25 14.30 0.30

**** 51 11.89 0.49

! Max uncertainty on the T is 2°C.

! Syntheses by 3 different methods. Isotopic equilibrium is considered reached in the majority of cases because of the coincidence of results for syntheses with different techniques.

_EX_	Vitali&al(2000)			2.04	-3.61	3.65	0	60	5
****	9	16.56	0.30						
****	24	14.59	0.69						
****	51	11.93	0.30						

! From precipitation of synthetic aluminum-hydroxide phases.

! Uncertainties on the T measurments 1°C at 9°C, 2°C at 24 and 51°C.

>> CALCITE/GIBBSITE			PURE			#3	TEST	<<------
_TH_	Zheng(1998)		0.12	3.86	-1.57	0	900	20

! Theoretical calculation by incremental method.

! Discrepanncy is observed between theoretical and experimental data (Bird et al., 1994) by the author. It may imply either that the theoretical calculations are in error for the mineral containing hydrogen bonds, or that the low-temperature calibrations by synthesis experiments have not provided reliable equilibrium fractionation factors.

>> QUARTZ/NORDSTRANDITE			PURE			#1	FIT	<<------
_TH_	Zheng(1998)		0.63	3.93	-1.64	0	900	20

! Theoretical calculation by incremental method.

>> NORDSTRANDITE/WATER			PURE			#2	TEST	<<------
_TH_	Zheng(1998)		3.85	-8.69	2.45	0	900	20

! Theoretical calculation by incremental method.

>> CALCITE/NORDSTRANDITE			PURE		#3	TEST	<<------	
_TH_	Zheng(1998)		0.16	4.03	-1.64	0	900	20

! Theoretical calculation by incremental method.

>> QUARTZ/BAYERITE			PURE			#1	FIT	<<------
_TH_	Zheng(1998)		0.67	4.08	-1.71	0	900	20

! Theoretical calculation by incremental method.

>> BAYERITE/WATER			PURE			#2	TEST	<<------
_TH_	Zheng(1998)		3.81	-8.85	2.48	0	900	20

! Theoretical calculation by incremental method.

>> CALCITE/BAYERITE			PURE			#3	TEST	<<------
_TH_	Zheng(1998)		0.20	4.18	-1.71	0	900	20

! Theoretical calculation by incremental method.

>> QUARTZ/LIMONITE		PURE			#1	FIT		<<------
_TH_	Zheng(1998)	0.52	3.48	-1.45	0	900	20	
! Theoretical calculation by incremental method.								
>> LIMONITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1998)	3.96	-8.24	2.37	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/LIMONITE		PURE			#3	TEST		<<------
_TH_	Zheng(1998)	0.05	3.58	-1.45	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/PYROCHROITE		PURE			#1	FIT		<<------
_TH_	Zheng(1998)	1.03	5.26	-2.22	0	900	20	
! Theoretical calculation by incremental method.								
>> PYROCHROITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1998)	3.45	-10.03	2.68	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/PYROCHROITE		PURE			#3	TEST		<<------
_TH_	Zheng(1998)	0.57	5.36	-2.22	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/SPERTINIITE		PURE			#1	FIT		<<------
_TH_	Zheng(1998)	0.91	4.91	-2.07	0	900	20	
! Theoretical calculation by incremental method.								
>> SPERTINIITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1998)	3.57	-9.67	2.63	0	900	20	
! Theoretical calculation by incremental method.								

>> CALCITE/SPERTINIITE PURE #3 TEST <<------

_TH_ Zheng(1998) 0.45 5.01 -2.07 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- OXIDES ---------- !!!!

>> QUARTZ/CASSITERITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 0.56 5.80 -3.04 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 0.83 4.65 -1.96 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_EX_ Zhang&al(1994) -6.87 26.29 -15.49 250 500 10

**** 500 6.9 0.2

**** 400 8.5 0.4

! The final equation was derived from the both the measured data and the combination of the data for cassiterite-water and the quartz-water calibration from Zhang&al(1989).

>> CASSITERITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 3.68 -9.58 2.00 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 3.65 -9.42 2.59 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_EX_ Zhang&al(1994) 10.13 -26.09 12.58 250 500 10

**** 370 -3.9 0.3

**** 310 -1.9 0.2

**** 250 -0.4 0.7

! Direct exchange between water and cassiterite recrystallized from amorphous SnO2 and synthesis of cassiterite from SnCl4*5H2O.

! Equilibrium assumed on the base of the strong consistency of the data from different experimental settings.

>> CALCITE/CASSITERITE PURE #3 TEST <<------

_TH_ Zheng(1991) 0.36 4.75 -1.96 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/CERIANITE PURE #1 FIT <<------

!_TH_	Zheng(1991)	1.67	9.32	-4.97	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Zheng(1991)	2.10	7.48	-3.21	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> CERIANITE/WATER	PURE			#2	TEST	<<------

!_TH_	Zheng(1991)	2.57	-13.09	3.93	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Zheng(1991)	2.38	-12.24	3.00	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/CERIANITE	PURE			#3	TEST	<<------

_TH_	Zheng(1991)	1.63	7.58	-3.21	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/CHROMITE	PURE			#1	FIT	<<------

!_TH_	Zheng(1991)	1.63	9.22	-4.91	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Zheng(1991)	2.05	7.39	-3.17	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> CHROMITE/WATER	PURE			#2	TEST	<<------

!_TH_	Zheng(1991)	2.62	-12.99	3.87	0	900	20	

! Theoretical calculation by incremental method.

_TH_	Zheng(1991)	2.43	-12.16	3.00	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/CHROMITE	PURE			#3	TEST	<<------

_TH_	Zheng(1991)	1.58	7.50	-3.17	0	900	20	

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/CORUNDUM	PURE			#1	FIT	<<------

!_TH_	Zheng(1991)	2.00	9.94	-3.45	0	900	20	

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.45 7.98 -1.96 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CORUNDUM/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.24 -13.71 4.28 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.03 -12.74 3.07 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/CORUNDUM PURE #3 TEST <<------

_TH_ Zheng(1991) 1.99 8.08 -3.45 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/FRANKLINITE PURE #1 FIT <<------

_TH_ Zheng(1991) 1.91 7.25 -3.11 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> FRANKLINITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1991) 2.52 -12.02 2.98 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/FRANKLINITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.49 7.35 -3.11 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> HEMATITE/WATER PURE #1 FIT <<------

!_TH_ Zheng(1991) 2.69 -12.82 3.78 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.52 -12.03 2.98 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_MX_ Clayton&Epstein(1961) 0.413 0.00 -2.56 25 120 5

! Based on natural co-existing quartz, calcite and hematite and experimental calcite-water of Clayton(1961).

_EX_ Yapp(1990) 1.63 0.00 -12.3 25 120 5

! Fractionation of hematite and geothite undistinguishable.

_EX_ Bao&Koch(1999) 0.73 0.00 -6.91 30 140 5

! Different from Yapp(1990) at T<95°C, according to the authors due to differences in the washing and drying protocols applied to the hematite precipitates.

>> QUARTZ/HEMATITE PURE #2 TEST <<------

!_TH_ Zheng(1991) 1.55 9.05 -4.82 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.96 7.26 -3.11 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/HEMATITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.50 7.36 -3.11 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/JACOBSITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.23 8.24 -4.37 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.61 6.61 -2.82 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> JACOBSITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 3.02 -12.02 3.33 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.87 -11.38 2.90 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/JACOBSITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.14 6.71 -2.82 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/MAGNESIOCHROMITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.76 9.49 -5.07 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.19 7.62 -3.28 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> MAGNESIOCHROMITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.48 -13.27 4.03 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.29 -12.38 3.03 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/MAGNESIOCHROMITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.73 7.72 -3.28 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/MAGNESIOFERRITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.29 8.43 -4.47 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.68 6.76 -2.89 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> MAGNESIOFERRITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.95 -12.20 3.43 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.80 -11.53 2.92 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/MAGNESIOFERRITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.22 6.86 -2.89 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/MAGNETITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.22 8.22 -4.35 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.60 6.59 -2.81 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_EX_ Matthews&al(1983a) 6.11 0.00 0.00 400 800 5

! Revised magnetite-water data of O'Neil(1963).

_MX_ Javoy&al(1970) 5.00 0.00 1.9 500 900 5

! Based on the experimental data from O'Neil&Clayton(1964), O'Neil&Taylor(1967), O'Neil&Taylor(1969).

! Based on literature data, but opposite trend with respect to all the other equations: QZ/MIN CALCULATED and not MIN/QZ.

! Changed from the original papaer (symmetric fit with respect to x axis).

!_NT_ Bottinga&Javoy(1975) 5.57 0.00 0.00 500 1100 5

! ! Data from Bottinga&Javoy(1973).

_NT_ Bottinga&Javoy(1975) 5.57 0.00 0.00 500 900 5

! Reduced T range.

_EX_ Chiba&al(1989) 6.29 0.00 0.00 200 900 5

! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).

! Fractionation data combined with the data of Clayton&al(1989).

! Standard error of the coefficient = 0.14.

>> MAGNETITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 3.02 -12.00 3.31 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.88 -11.36 2.89 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

!_MX_ Bottinga&Javoy(1973) 1.19 -0.88 2.17 500 800 5

! ! Limited laboratory measurements Anderson&al(1971) do not agree with the theoretical relation.

! ! No data on the anharmonicity of the magnetite lattice vibrations was known (therefore, the same strategy used to calculated the parameters for anhydrous crystalline silicates was applied).

! ! Pramaters corrected by Friedman&O'Neil(1977).

_MX_ Bottinga&Javoy(1973) -1.47 0.00 -3.70 500 800 5

! Pramaters corrected by Friedman&O'Neil(1977).

_MX_ Becker&Clayton(1976) 2.71 -11.55 3.73 0 727 5

! Parameters recalculated by polynomial regression of the point data given in the paper. R^2=0.9982.

! Calculation was done by based on theoretical considerations by Urey(1947) and by Bigeleisen&Mayer(1947).

>> CALCITE/MAGNETITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.13 6.70 -2.81 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

!_EX_ Chiba&al(1989) 3.29 0.00 0.00 200 1200 5

!**** 800 5.20 0.14
!**** 1000 3.59 0.14
!**** 1200 2.68 0.14
! ! P = 15- 16 kbar. Carbonate-exchange technique of Clayton&al(1989).
! ! Fractionation data combined with the data of Clayton&al(1989).
! ! Correlation coefficient = 0.999.
! ! Standard error of the coefficient = 0.12.

_EX_ Chiba&al(1989) 3.29 0.00 0.00 200 900 5
  ! Reduced T range.

>> QUARTZ/PEROVSKITE PURE #1 FIT <<------

!_EX_ Chacko&al(2001) 6.80 0.00 0.00 800 1000 5
! ! Recalculated from calcite-perovskite of Gautason&al(1993).

_EX_ Chacko&al(2001) 6.80 0.00 0.00 800 900 5
  ! Reduced T range.

>> CALCITE/PEROVSKITE PURE #3 TEST <<------

!_EX_ Gautason&al(1993) 6.42 0.00 0.00 800 1000 5
! ! Direct exchange at P=15 kbar.

_EX_ Gautason&al(1993) 6.42 0.00 0.00 800 900 5
  ! Reduced T range.

>> QUARTZ/PLATTNERITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 0.56 5.8 -3.04 0 900 20
  ! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 0.83 4.65 -1.96 0 900 20
  ! Theoretical calculation by incremental method (revised, Table 2).

>> PLATTNERITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 3.68 -9.58 2.00 0 900 20
  ! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 3.65 -9.42 2.59 0 900 20
  ! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/PLATTNERITE PURE #3 TEST <<------

_TH_ Zheng(1991) 0.36 4.75 -1.96 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/PYROLUSITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 0.64 6.16 -3.23 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 0.92 4.94 -2.08 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> PYROLUSITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 3.61 -9.94 2.19 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 3.56 -9.71 2.63 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/PYROLUSITE PURE #3 TEST <<------

_TH_ Zheng(1991) 0.46 5.04 -2.08 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/RUTILE PURE #1 FIT <<------

!_TH_ Zheng(1991) 0.79 6.82 -3.59 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 1.11 5.47 -2.31 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_EX_ Matthews&Schliestedt(1984) 4.54 0.00 0.00 500 700 5

! Based on the experimental Rt-H2o and Qtz-H2O calibrations of Matthews&al(1979) and Matsuhisa&al(1979), reviwed to be consistent with Bottinga&Javoy(1973) prediction of a zero intercept.

_EX_ Addy&Garlick(1974) 6.6 0.00 -2.9 575 775 5

! Combination of their results with the hydrothermal quartz-water calibration of Clayton&al(1972).

! No isotopic exchange between Rt and H2O at T << 600°C.

_EX_ Matthews&al(1979) 7.23 0.00 -3.08 500 700 5

! Combination of their results with the hydrothermal quartz-water calibration of Clayton&al(1972).

_NT_ Agrinier(1991) 4.78 0.00 0.00 450 800 5

**** 460 9.1 0.225

**** 485 7.4 0.225

****	510	7.2	0.225
****	520	6.9	0.225
****	530	7.2	0.225
****	530	6.8	0.225
****	540	6.9	0.225
****	540	7.3	0.225
****	565	6.2	0.225
****	570	6.5	0.225
****	575	7.7	0.225
****	580	6.5	0.225
****	590	7.3	0.225
****	590	6.4	0.262
****	590	6.5	0.262
****	620	6.5	0.150
****	655	6.0	0.225
****	725	4.7	0.262
****	730	5.0	0.300
****	800	4.3	0.262

! Uncertainty on the A coefficient was calculated at 0.08.

! References for the natural samples are reported in the paper.

_MX_	Matthews(1994)	5.02	0.00	0.00	400	700	5

! Combining min-water data with quartz-water data from Matsuhisa&al(1979).

_EX_	Chacko&al(2001)	4.69	0.00	0.00	500	800	5

! Recalculated from Chacko&al(1996).

>> RUTILE/WATER		PURE			#2	TEST	<<------
!_TH_	Zheng(1991)	3.45	-10.6	2.55	0	900	20

! Theoretical calculation by incremental method.

_TH_	Zheng(1991)	3.37	-10.23	2.72	0	900	20

! Theoretical calculation by incremental method (revised, Table 2).

!_EX_	Addy&Garlick(1974)	-4.10	0.00	0.96	575	775	5
!****	775	-2.8	0.00				
!****	675	-3.5	0.00				
!****	575	-4.8	0.00				

! ! SD of the experimental points is 0 because no data is available in the paper.

! ! Exchange by crystallization of amorphous TiO2 powder.

! ! Pramaters corrected by Friedman&O'Neil(1977).

_EX_	Addy&Garlick(1974)	-4.10	0.00	1.46	575	775	5

! Pramaters corrected by Friedman&O'Neil(1977).

_EX_	Matthews&al(1979)	-4.72	0.00	1.62	500	700	5
****	304	-6.20	0.125				
****	405	-6.64	0.135				

**** 508 -6.11 0.08

**** 608 -4.45 0.14

**** 698 -3.38 0.075

! Exchange by controlled oxidation of Ti metal powder under hydrothermal conditions.

! Mean and SD are calculated in the paper. Here the uncertainty on the T value is not reported.

! The T range is chosen between 500 and 700 °C because the proposed equation fits properly only the 3 experiments at 508,608 and 698 °C.

! The low-T data might require a more complex function (T^4) to be fit.

_MX_ Bird&al(1994) 1.62 0.00 -12.53 22 50 15

**** 22 6.68 0.60

**** 50 2.30 1.00

! Attainment of isotopic equilibrium cannot be proven. Good concordance of results from different experimental settings and with experimental samples.

>> CALCITE/RUTILE PURE #3 TEST <<------

_TH_ Zheng(1991) 0.64 5.57 -2.31 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

_EX_ Matthews(1994) 4.64 0.00 0.00 400 700 5

! Combining min-water data with quartz-water data from Matsuhisa&al(1979).

_EX_ Chacko&al(2001) 4.31 0.00 0.00 500 800 5

! Data from Chacko&al(1996).

>> QUARTZ/THORIANITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.66 9.30 -4.96 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.09 7.46 -3.21 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> THORIANITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.58 -13.07 3.92 0 900 20

! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.39 -12.23 3.02 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> CALCITE/THORIANITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.62 7.56 -3.21 0 900 20

! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/URANINITE PURE #1 FIT <<------

!_TH_ Zheng(1991) 1.61 9.19 -4.90 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.03 7.37 -3.17 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> URANINITE/WATER PURE #2 TEST <<------

!_TH_ Zheng(1991) 2.63 -12.97 3.86 0 900 20
! Theoretical calculation by incremental method.

_TH_ Zheng(1991) 2.45 -12.14 3.00 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

!_EX_ Fayek&Kyser(2000) 16.58 -77.52 77.48 100 300 5
! ! Exchange experiments with CO2.Interpolation of 3 points with an uncertainty at 2.5 permil (2SD).

>> CALCITE/URANINITE PURE #3 TEST <<------

_TH_ Zheng(1991) 1.57 7.48 -3.17 0 900 20
! Theoretical calculation by incremental method (revised, Table 2).

>> QUARTZ/WOLFRAMITE PURE #1 FIT <<------

_TH_ Zheng(1992) 0.38 4.76 -2.48 0 900 20
! Theoretical calculation by incremental method.

EX_ Zhang&al(1994) -1.04 10.74 -6.27 200 420 10
! Calculated by combining the experimantal data on wolframite-water with the quartz-water calibration from Zhang&al(1989).

>> WOLFRAMITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1992) 3.86 -8.54 1.44 0 900 20
! Theoretical calculation by incremental method.

_EX_ Zhang&al(1994) 3.13 -6.42 -0.12 200 420 10
**** 420 -2.8 0.3
**** 370 -2.6 0.5
**** 310 -2.1 0.4
**** 250 -1.1 0.4
**** 200 0.4 0.7
! Wolframite syntetized with ferberite and huebnerite in solutions 0 to 30 wt% NaCl or NaF.
! Hydrothermal pressures between 300 and 800 bars.

! Equilibrium assumed on the base of the strong consistency of the data from different experimental settings.

!!!! ---------- !!!!

!!!! ---------- FELDSPATHOID ---------- !!!!

>> LEUCITE/WATER		PURE			#1	FIT		<<------
_TH_	Zheng(1993a)	4.26	-6.67	2.08	0	900	20	

! Theoretical calculation by incremental method.

>> QUARTZ/LEUCITE		PURE			#2	TEST		<<------
_TH_	Zheng(1993a)	0.22	1.91	-0.79	0	900	20	

! Theoretical calculation by incremental method.

>> CALCITE/LEUCITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993a)	-0.24	2.01	-0.79	0	900	20	

! Theoretical calculation by incremental method.

>> NEPHELINE/WATER		PURE			#1	FIT		<<------
_TH_	Zheng(1993a)	4.11	-7.53	2.24	0	900	20	

! Theoretical calculation by incremental method.

>> QUARTZ/NEPHELINE		PURE			#2	TEST		<<------
_TH_	Zheng(1993a)	0.37	2.77	-1.15	0	900	20	

! Theoretical calculation by incremental method.

>> CALCITE/NEPHELINE		PURE			#3	TEST		<<------
_TH_	Zheng(1993a)	-0.1	2.89	-1.15	0	900	20	

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- PYROXENOIDS ---------- !!!!

>> QUARTZ/PECTOLITE		PURE			#1	FIT		<<------

_TH_ Zheng(1993b) 0.41 2.95 -1.23 0 900 20

! Theoretical calculation by incremental method.

>> PECTOLITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 4.08 -7.71 2.28 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/PECTOLITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.06 3.05 -1.23 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/RHODONITE PURE #1 FIT <<------

_TH_ Zheng(1993a) 0.63 3.94 -1.65 0 900 20

! Theoretical calculation by incremental method.

>> RHODONITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 3.85 -8.71 2.46 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/RHODONITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.16 4.04 -1.65 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- SULFATES ---------- !!!!

>> ALUNITE/WATER PURE #1 FIT <<------

_EX_ Stoffregen&al(1994) 3.09 0.00 -2.94 250 450 5

**** 450 1.9 0.3

**** 400 3.8 0.3

**** 350 4.5 0.3

! Cation exchange experiments. 8-95% exchange.

! Equation for ALUNITE(SO4).

```
_EX_        Stoffregen&al(1994)                2.28    0.00    -3.90          250     450     5
****        450     1.2     0.4
****        400     -0.20   0.4
****        400     1.3     0.4
****        350     1.7     0.4
     ! Cation exchange experiments. 8-95% exchange.
     ! Equation for ALUNITE(OH).

>> ANGLESITE/WATER                           PURE                           #1      FIT             <<------

_TH_        Zheng(1999)                        3.94    -5.54   1.87           0       900     20
     ! Theoretical calculation by incremental method.
     ! Corrected from Table 4 in the reference paper.

>> QUARTZ/ANGLESITE                          PURE                           #2      TEST            <<------

_TH_        Zheng(1999)                        0.54    0.78    -0.36          0       900     20
     ! Theoretical calculation by incremental method.
     ! Corrected from Table 4 in the reference paper.

>> ANHYDRITE/WATER                           PURE                           #1      FIT             <<------

_TH_        Zheng(1999)                        4.19    -4.59   1.71           0       900     20
     ! Theoretical calculation by incremental method.
     ! Corrected from Table 4 in the reference paper.

!_EX_        Lloyd(1968)                        3.878   0.00    -3.40          100     500     10
!    ! P = 690 bars.
!    ! Parameters were corrected by Freidman&O'Neil(1977).

_EX_        Lloyd(1968)                        3.88    0.00    -2.90          100     500     10
     ! Parameters corrected by Freidman&O'Neil(1977).

_EX_        Chiba&al(1981)                     3.21    0.00    -4.72          100     550     10
     ! Direct exchange in water 1m NaCl.
     ! P = 1-1000 bars.

!>> QUARTZ/ANHYDRITE                         PURE                           #2      TEST            <<------
!
!_TH_        Zheng(1999)                        0.29    -0.17   0.05           0       900     20
!    ! Theoretical calculation by incremental method.
!    ! Corrected from Table 4 in the reference paper.

>> BARITE/WATER                              PURE                           #1      FIT             <<------
```

_TH_ Zheng(1999) 3.94 -5.47 1.86 0 900 20

! Theoretical calculation by incremental method.

! Corrected from Table 4 in the reference paper.

!_EX_ Kusakabe&Robinson(1977) 2.64 0.00 -5.3 110 350 10

!**** 350 1.84 0.10

!**** 300 2.90 0.24

!**** 250 4.53 0.13

!**** 250 5.19 0.43

!**** 200 6.50 0.10

!**** 150 10.33 0.91

!**** 110 12.73 1.52

! ! Direct exchange in solution 1m NaCl, HCl or H2SO4.

! ! 28-98% exchange.

! ! P = 1-1000 bars.

_EX_ Kusakabe&Robinson(1977) 3.01 0.00 -7.3 110 350 10

**** 350 1.84 0.10

**** 300 2.90 0.24

**** 250 4.53 0.13

**** 250 5.19 0.43

**** 200 6.50 0.10

**** 150 10.33 0.91

**** 110 12.73 1.52

! data corrected for ion hydration effects in solution.

>> QUARTZ/BARITE PURE #2 TEST <<------

_TH_ Zheng(1999) 0.54 0.71 -0.33 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- SERPENTINE ---------- !!!!

>> AMESITE/WATER CHLORITE #1 FIT <<------

_TH_ Zheng(1993b) 3.95 -8.3 2.38 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.54 -1.10 -1.9 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/AMESITE CHLORITE #2 TEST <<------

_TH_ Zheng(1993b) 0.53 3.53 -1.47 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/AMESITE CHLORITE #3 TEST <<------

_TH_ Zheng(1993b) 0.06 3.63 -1.47 0 900 20

! Theoretical calculation by incremental method.

>> CHRYSOTILE/WATER PURE #1 FIT <<------

_TH_ Richter&Hoernes(1988) 0.08 -1.01 -2.01 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/LIZARDITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.51 3.42 -1.43 0 900 20

! Theoretical calculation by incremental method.

>> LIZARDITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 3.97 -8.19 2.36 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/LIZARDITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.04 3.52 -1.43 0 900 20

! Theoretical calculation by incremental method.

>> SERPENTINE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 3.99 -8.12 2.35 0 900 20

! Theoretical calculation by incremental method.

_NT_ Wenner&Taylor(1971) 1.56 0.00 -4.70 150 400 5

! Parameters from Chacko&al(2001).

_NT_ Früh-Green&al(1996) 1.51 0.00 -4.57 150 400 5

! Obtained by using the empirical Qtz-H2O calibration by Sharp&Kirschner(1994) and Srp-Mag data.

>> QUARTZ/SERPENTINE PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.49 3.35 -1.40 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/SERPENTINE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.02 3.45 -1.40 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- CLAY MINERALS ---------- !!!!

>> QUARTZ/ILLITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.34 2.6 -1.08 0 900 20
! Theoretical calculation by incremental method.

_NT_ Eslinger&Savin(1973) 0.95 0.00 0.88 160 270 5
! Study on hydrothermally altered volcanic rocks.

>> ILLITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993b) 4.14 -7.36 2.21 0 900 20
! Theoretical calculation by incremental method.

_MX_ Savin&Lee(1988) 2.39 0.00 -4.19 160 270 5
! Based on the natural sample quartz-illite curve of Eslinger&Savin(1973) and the quartz-H2O curve of Matsuhisa&al(1979).
! T from Eslinger&Savin(1973).

_MX_ Sheppard&Gilg(1996) 2.39 0.00 -3.76 0 350 5
! Based on the natural sample and cation exchange experiments on muscovite by O'Neil& Taylor(1969).

>> CALCITE/ILLITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.13 2.70 -1.08 0 900 20
! Theoretical calculation by incremental method.

>> QUARTZ/KAOLINITE PURE #1 FIT <<------

_TH_ Zheng(1993b) 0.19 1.68 -0.69 0 900 20
! Theoretical calculation by incremental method.

>> KAOLINITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	4.29	-6.44	2.03	0	900	20	
! Theoretical calculation by incremental method.								
_MX_	Sheppard&Gilg(1996)	2.76	0.00	-6.75	0	350	5	
! Based on the natural sample and a experimental data by Kulla(1978).								
_TH_	Richter&Hoernes(1988)	1.88	-0.64	-2.46	300	800	20	
! Water parameters are taken from experimental data from the literature (not specified).								
! An "average qtz-water curve" forms the basis for the increment method calculation.								
_MX_	Eslinger(1971)	2.5	0.00	-2.87	0	350	5	
! Reference in Cacko&al(2001).								
! Combination of natural data and model calculations.								
_EX_	Kulla(1978)	2.42	0.00	-4.45	170	320	5	
! Hydrothermal synthesis of kaolinite from gels.								
>> CALCITE/KAOLINITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	-0.28	1.78	-0.69	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/PYROPHYLLITE		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.08	0.86	-0.35	0	900	20	
! Theoretical calculation by incremental method.								
>> PYROPHYLLITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	4.40	-5.62	1.87	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/PYROPHYLLITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	-0.38	0.96	-0.35	0	900	20	
! Theoretical calculation by incremental method.								
>> SMECTITE/WATER		PURE			#1	FIT		<<------
_MX_	Sheppard&Gilg(1996)	2.55	0.00	-4.05	0	350	5	

! Based on the natural sample and a experimental data by Kulla(1979).

_MX_ Savin&Lee(1988) 2.58 0.00 4.19 0 350 5

! Modification of the equation of Yeh&Savin(1977).

! Based on analysis of authigenic smecite formed at 1°C, natural smectite-illite pairs, quartz-illite curve of Eslinger&Savin(1973), quartz-H2O curve of Matsuhisa&al(1979).

_EX_ Escande&al(1984) 3.31 0.00 -4.82 25 95 20

! In Chacko&al(2001).

! Synthesis of Mg-rich smectite under hydrothermal conditions. The technique of analyzing smectites may have resulted in an overestimation of the fractionation factor (Savin&Lee, 1988).

>> TALC/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 4.2 -7.04 2.14 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.26 -0.85 -2.20 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/TALC PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.28 2.27 -0.94 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/TALC PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.19 2.38 -0.94 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.25 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- TITANITE GRUOP ---------- !!!!

>> MALAYAITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993a) 3.88 -8.60 2.43 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/MALAYAITE PURE #2 TEST <<------

_TH_ Zheng(1993a) 0.60 3.83 -1.60 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/MALAYAITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.14 3.94 -1.60 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/TITANITE PURE #1 FIT <<------

_TH_ Zheng(1993a) 0.67 4.11 -1.72 0 900 20

! Theoretical calculation by incremental method.

!_NT_ King&al(2001) 3.57 0.00 0.00 450 1000 5

! ! Equation in constrast with the incremental method results.

_NT_ King&al(2001) 3.57 0.00 0.00 450 900 5

! Reduced T range.

_TH_ Hoffbauer&al(1994) 2.75 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

>> TITANITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 3.81 -8.87 2.49 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.12 -0.90 -2.14 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/TITANITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.21 4.21 -1.72 0 900 20

! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.375 0.00 0.00 600 900 20

! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).

!!!! ---------- !!!!

!!!! ---------- PHENACITE GROUP ---------- !!!!

>> PHENACITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993a) 3.42 -10.11 2.70 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/PHENACITE PURE #2 TEST <<------

_TH_ Zheng(1993a) 1.06 5.34 -2.26 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/PHENACITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.60 5.45 -2.26 0 900 20

! Theoretical calculation by incremental method.

>> WILLEMITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993a) 3.79 -8.94 2.50 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/WILLEMITE PURE #2 TEST <<------

_TH_ Zheng(1993a) 0.69 4.18 -1.75 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/WILLEMITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.23 4.28 -1.75 0 900 20

! Theoretical calculation by incremental method.

!!!! ---------- !!!!

!!!! ---------- ZIRCON GROUP ---------- !!!!

>> THORITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993a) 3.69 -9.27 2.55 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/THORITE PURE #2 TEST <<------

_TH_ Zheng(1993a) 0.79 4.50 -1.89 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/THORITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.32 4.61 -1.89 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/ZIRCON PURE #1 FIT <<------

_TH_ Zheng(1993a) 0.72 4.26 -1.79 0 900 20

! Theoretical calculation by incremental method.

_NT_ Valley&al(2003) 2.64 0.00 0.00 650 900 5

! Uncertainty on the A coefficient was calculated at 0.08 (1SD).

! No T range validity given; here the range of the natural data was chosen.

! In Fig.2 in the paper extrapolation for T > 500 °C.

!_EX_ Krylov&al(2002) 1.36 0.00 0.00 700 900 5

!**** 700 1.42 0.15

!**** 800 1.17 0.10

!**** 900 1.05 0.19

!**** 900 1.13 0.18

!**** 1000 0.85 0.12

!**** 1000 0.75 0.14

! ! Experimental data are recalculated from ZRN-H2O fractionation experiments using QTZ-H2O fractionation parameters from Bottinga&Javoy(1973). 1 standard error on the mean for ZRN-H2O couple.

! ! R^2 of the interpolation = 0.97.

! ! Synthesis experiment. Possible problems related to the kinetics of isotope exchange reactions and difficulty of attaining and preserving equilibrium discussed by the authors.

!_EX_ Trail&al(2009) 2.33 0.00 0.00 700 1000 5

! ! P = 10-20 kbar. Oxygen fugacity buffered in come experiments.

! ! Synthesized quartz and zircon in the presence of aqueous fluid in a piston-cylinder apparatus.

_EX_ Trail&al(2009) 2.33 0.00 0.00 700 900 5

! Reduced T range.

>> ZIRCON/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 3.76 -9.03 2.52 0 900 20

! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.81 -0.66 -2.43 300 800 20

! Water parameters are taken from experimental data from the literature (not specified).

! An "average qtz-water curve" forms the basis for the increment method calculation.

!_EX_ Krylov&al(2002) 2.74 0.00 -3.70 700 1000 5

!**** 700 -0.79 0.15

!**** 800 -1.31 0.10

!**** 900 -1.77 0.19

!**** 900 -1.85 0.18

!**** 1000 -2.02 0.12

!**** 1000 -1.93 0.14

! ! Experimental data are average on the splits of one experiment ± 1 standard error on the mean.

! ! R^2 of the interpolation = 0.97.

! ! Synthesis experiment. Possible problems related to the kinetics of isotope exchange reactions and difficulty of attaining and preserving equilibrium discussed by the authors.

!!!! ---------- SINGLE PHASES ---------- !!!!

>> AXINITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 4.20 -7.02 2.15 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/AXINITE PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.28 2.26 -0.94 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/AXINITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.19 2.36 -0.94 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/BERYL PURE #1 FIT <<------

_TH_ Zheng(1993a) 0.50 3.40 -1.42 0 900 20

! Theoretical calculation by incremental method.

>> BERYL/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 3.98 -8.16 2.34 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/BERYL PURE #3 TEST <<------

_TH_ Zheng(1993a) -0.03 3.50 -1.42 0 900 20

! Theoretical calculation by incremental method.

>> DATOLITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 4.33 -6.21 1.99 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/DATOLITE PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.15 1.44 -0.60 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/DATOLITE PURE #3 TEST <<------

_TH_ Zheng(1993b) -0.31 1.54 -0.60 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/GEHLENITE PURE #1 FIT <<------

_EX_ Chacko&al(2001) 3.50 0.00 0.00 800 1000 5

! Recalculated from experimental data of Chacko&al(1996).

! T not specified by the authors.

>> CALCITE/GEHLENITE PURE #2 TEST <<------

_EX_ Chacko&al(2001) 3.12 0.00 0.00 800 900 5

! Recalculated from experimental data of Chacko&al(1996).

! T not specified by the authors.

>> ILVAITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 3.43 -10.08 2.69 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/ILVAITE PURE #2 TEST <<------

_TH_ Zheng(1993b) 1.05 5.32 -2.24 0 900 20

! Theoretical calculation by incremental method.

>> CALCITE/ILVAITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.58 5.42 -2.24 0 900 20

! Theoretical calculation by incremental method.

>> QUARTZ/LAWSONITE PURE #1 FIT <<------

_NT_	Taylor&Coleman(1968)	1.64	0.00	1.47	150	400	5	
>> QUARTZ/PREHNITE		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.30	2.40	-1.00	0	900	20	
! Theoretical calculation by incremental method.								
>> PREHNITE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	4.18	-7.17	2.18	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/PREHNITE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	0.17	2.50	-1.00	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/TOURMALINE		PURE			#1	FIT		<<------
_TH_	Zheng(1993b)	0.27	2.22	-0.92	0	900	20	
! Theoretical calculation by incremental method.								
_NT_	Kotzer&al(1993)	1.00	0.00	0.39	200	600	5	
! Uncertainty on A = 0.17, uncertainty on B = 0.44.								
_NT_	Matthews&al(2003)	1.70	0.00	0.00	400	700	5	
>> TOURMALINE/WATER		PURE			#2	TEST		<<------
_TH_	Zheng(1993b)	4.21	-6.99	2.14	0	900	20	
! Theoretical calculation by incremental method.								
>> CALCITE/TOURMALINE		PURE			#3	TEST		<<------
_TH_	Zheng(1993b)	-0.20	2.32	-0.92	0	900	20	
! Theoretical calculation by incremental method.								
>> QUARTZ/WOLLASTONITE		PURE			#1	FIT	<<------	
_TH_	Zheng(1993a)	0.67	4.11	-1.72	0	900	20	
! Theoretical calculation by incremental method.								

_EX_ Matthews&al(1983a) 2.2 0.00 0.00 400 800 5

>> WOLLASTONITE/WATER PURE #2 TEST <<------

_TH_ Zheng(1993a) 3.81 -8.87 2.49 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 1.19 -0.88 -2.17 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> CALCITE/WOLLASTONITE PURE #3 TEST <<------

_TH_ Zheng(1993a) 0.21 4.21 -1.72 0 900 20
! Theoretical calculation by incremental method.

_TH_ Hoffbauer&al(1994) 2.30 0.00 0.00 600 900 20
! Calculation based on fractionation coefficients for Qtz-Cal and An-Cal of Chiba&al(1989).
! Parameters for Mg-Biotite with Mg4Al1.67.

>> VESUVIANITE/WATER PURE #1 FIT <<------

_TH_ Zheng(1993b) 3.55 -9.74 2.63 0 900 20
! Theoretical calculation by incremental method.

_TH_ Richter&Hoernes(1988) 0.28 -1.20 -1.79 300 800 20
! Water parameters are taken from experimental data from the literature (not specified).
! An "average qtz-water curve" forms the basis for the increment method calculation.

>> QUARTZ/VESUVIANITE PURE #2 TEST <<------

_TH_ Zheng(1993b) 0.93 4.97 -2.09 0 900 20
! Theoretical calculation by incremental method.

>> CALCITE/VESUVIANITE PURE #3 TEST <<------

_TH_ Zheng(1993b) 0.47 5.07 -2.09 0 900 20
! Theoretical calculation by incremental method.

!!!! ---------- !!!!