Materials for inclusion in GSA Data Repository

The following pages include three different data sets for inclusion in the data repository as follows:

Table DR1 - Summary of mineral chemistry and electron microprobe analyses of the samples reported here.

Table DR2 - Complete tables of Thermocalc results for each of the samples investigated here. In most cases the results of multiple runs are included to illustrate the effects of varying water activity or including or excluding selected mineral phases that may not have reached equilibrium with the rest of the assemblage.

Figure DR1 to DR19 - Zoning profiles for garnet porphyroblasts from each sample.

Table DR1 – Mineral rim Compositional Data

Average electron microprobe analyses of garnet rims.

Sample	AL1	GP1	GP2	SC1	SC2
SiO2	37.32	37.35	36.94	37.65	37.71
TiO2	0.00	0.00	0.00	0.00	0.00
Al2O3	21.21	21.13	20.94	21.44	21.39
Fe2O3	0.28	0.09	0.52	0.23	0.17
FeO	30.75	35.68	33.70	32.97	31.59
MnO	7.82	1.92	5.79	1.96	1.74
MgO	2.38	3.12	2.24	3.59	3.69
CaO	1.21	1.31	1.74	3.32	3.91
sum	100.97	100.60	101.87	101.16	100.20
		Cations on the Basis of 12 Oxygen			
Si	2.99	2.99	2.96	2.98	3.00
Al	0.01	0.01	0.04	0.02	0.00
sum	3.00	3.00	3.00	3.00	3.00
Al	2.00	1.99	1.94	1.98	2.00
Fe+++	0.02	0.01	0.03	0.01	0.01
Ti	0.00	0.00	0.00	0.00	0.00
sum	2.02	2.00	1.97	2.00	2.01
Ca	0.10	0.11	0.15	0.28	0.33
Fe++	2.06	2.39	2.26	2.18	2.10
Mg	0.28	0.37	0.27	0.42	0.44
Mn	0.53	0.13	0.39	0.13	0.12
sum	2.98	3.01	3.07	3.02	2.99
X(Alm)	0.69	0.80	0.74	0.72	0.70
X (Py)	0.10	0.12	0.09	0.14	0.15
X(Sp)	0.18	0.04	0.13	0.04	0.04
X(Gr)	0.03	0.04	0.05	0.09	0.11

Table DR1 (cont.) Average electron microprobe analyses of garnet rims.

Sample	WL1	WL2A	WL2B	WL3	LB1	LB2
SiO2	37.50	38.26	38.20	37.59	37.38	37.33
TiO2	0.00	0.00	0.04	0.00	0.00	0.00
Al2O3	21.09	21.74	21.19	21.36	20.98	21.35
Fe2O3	0.25	0.75	1.74	0.15	0.39	0.12
FeO	34.46	29.16	26.94	32.65	36.15	35.38
MnO	2.25	0.81	1.20	3.28	2.94	1.13
MgO	2.88	6.83	7.45	3.61	2.44	4.25
CaO	1.82	2.81	3.34	1.94	1.15	0.80
sum	100.25	100.36	100.10	100.58	101.43	100.36
		Cations on the Basis of 12 Oxygen				
Si	3.01	2.98	2.97	2.99	2.99	2.98
Al	0.00	0.02	0.03	0.01	0.01	0.02
sum	3.01	3.00	3.00	3.00	3.00	3.00
Al	2.00	1.98	1.92	2.00	1.97	1.99
Fe+++	0.02	0.04	0.10	0.01	0.02	0.01
Ti	0.00	0.00	0.00	0.00	0.00	0.00
sum	2.01	2.02	2.02	2.01	2.00	2.00
Ca	0.16	0.24	0.28	0.17	0.10	0.07
Fe++	2.31	1.90	1.75	2.18	2.42	2.36
Mg	0.34	0.79	0.86	0.43	0.29	0.51
Mn	0.15	0.05	0.08	0.22	0.20	0.08
sum	2.97	2.98	2.98	2.99	3.01	3.01
X(Alm)	0.78	0.64	0.59	0.73	0.80	0.78
X (Py)	0.12	0.27	0.29	0.14	0.10	0.17
X(Sp)	0.05	0.02	0.03	0.07	0.07	0.03
X(Gr)	0.05	0.08	0.09	0.06	0.03	0.02

Table DR1 (cont.) Average electron microprobe analyses of biotite and muscovite.

Sample	AL1 (Bt)	AL1 (Mu)	GP1 (Bt)	GP2 (Bt)	GP2 (Mu)	SC1(Bt)	SC2 (Bt)
SiO2	34.44	44.40	35.58	34.99	46.74	35.08	36.16
TiO2	2.69	0.56	2.36	2.80	0.10	2.17	2.74
Al2O3	20.33	36.52	20.79	20.44	37.87	20.81	20.67
FeO	20.24	1.58	21.07	21.03	1.41	21.93	17.94
MnO	0.23	0.01	0.08	0.20	0.02	0.14	0.12
MgO	7.44	0.51	7.47	6.13	0.60	7.54	9.76
CaO	0.00	0.00	0.02	0.03	0.00	0.01	0.02
Na2O	0.19	0.37	0.23	0.19	0.41	0.25	0.17
K2O	9.35	9.87	8.96	9.07	9.43	9.00	9.00
sum	94.91	93.82	96.56	94.88	96.58	96.93	96.58
Cations on the Basis of 12 Oxygen							
Si	2.65	3.00	2.68	2.69	3.01	2.64	2.68
Al	1.36	1.00	1.32	1.31	0.99	1.36	1.32
sum	4.00	4.00	4.00	4.00	4.00	4.00	4.00
Al	0.49	1.90	0.52	0.54	1.89	0.49	0.48
Ti	0.16	0.03	0.13	0.16	0.05	0.12	0.15
Fe	1.30	0.09	1.33	1.35	0.08	1.38	1.11
Mn	0.02	0.00	0.01	0.01	0.00	0.01	0.01
Mg	0.85	0.05	0.84	0.70	0.06	0.85	1.08
sum	2.81	2.07	2.82	2.77	2.07	2.86	2.83
Ca	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na	0.03	0.05	0.03	0.03	0.05	0.04	0.02
K	0.92	0.85	0.86	0.89	0.78	0.87	0.85
sum	0.95	0.90	0.90	0.92	0.83	0.90	0.88
X(Al)	0.17	0.92	0.18	0.19	0.91	0.17	0.17
X(Ti)	0.06	0.01	0.05	0.06	0.02	0.04	0.05
X(Fe)	0.46	0.04	0.47	0.49	0.04	0.48	0.39
X(Mg)	0.30	0.02	0.30	0.25	0.03	0.30	0.38

Table DR1 (cont.) Average electron microprobe analyses of biotite.

Sample	WL1 (Bt)	WL2A (Bt)	WL2B (Bt)	WL3 (Bt)	LB1 (Bt)	LB2 (Bt)
SiO2	35.37	36.73	36.85	35.55	34.67	35.88
TiO2	3.55	1.08	1.14	3.21	3.81	2.01
Al2O3	19.23	18.48	17.94	18.97	20.61	19.87
FeO.	22.33	14.69	15.68	19.42	22.10	19.22
MnO	0.06	0.73	0.80	0.10	0.11	0.02
MgO	7.85	14.98	15.02	9.42	5.93	9.89
CaO	0.00	0.02	0.04	0.00	0.01	0.01
Na2O	0.16	0.86	0.67	0.15	0.20	0.34
K2O	9.45	7.47	7.76	8.94	9.32	8.81
sum	98.00	95.04	95.90	95.76	96.76	96.05
		Cations on the Basis of 12 Oxygen				
Si	2.65	2.72	2.72	2.68	2.63	2.69
Al	1.35	1.28	1.28	1.32	1.37	1.31
sum	4.00	4.00	4.00	4.00	4.00	4.00
Al	0.35	0.33	0.28	0.37	0.47	0.45
Ti	0.20	0.06	0.06	0.18	0.22	0.11
Fe	1.40	0.91	0.91	1.23	1.40	1.21
Mn	0.00	0.05	0.05	0.01	0.01	0.00
Mg	0.88	1.65	1.65	1.06	0.67	1.11
sum	2.83	3.00	2.95	2.85	2.76	2.87
Ca	0.00	0.00	0.00	0.00	0.00	0.00
Na	0.02	0.12	0.10	0.02	0.03	0.05
K	0.91	0.71	0.73	0.86	0.90	0.84
sum	0.93	0.83	0.83	0.88	0.93	0.89
X(Al)	0.12	0.11	0.09	0.13	0.17	0.16
X(Ti)	0.07	0.02	0.02	0.06	0.08	0.04
X(Fe)	0.49	0.30	0.31	0.43	0.51	0.42
X(Mg)	0.31	0.55	0.56	0.37	0.24	0.39

Table DR1 (cont). Average electron microprobe analyses of plagioclase and potassium feldspar.

Samples	AL1 (Pl)	AL1 (Ks)	GP2 (Pl)	SC1 (Pl)	SC2 (Pl)	WL1 (Pl)	WL1 (Ks)
SiO2	62.54	64.91	60.78	61.72	58.58	61.31	64.61
Al2O3	24.60	19.35	25.29	25.31	26.85	24.08	19.36
Fe2O3	0.03	0.05	0.04	0.11	0.08	0.17	0.02
CaO	4.91	0	5.87	5.57	7.78	4.88	0
Na2O	9.35	2.03	8.71	8.62	6.86	8.71	1.91
K2O	0.25	13.77	0.2	0.12	0.11	0.24	13.79
sum	101.68	100.11	100.89	101.45	100.26	99.39	99.69
Cations on the Basis of 8 Oxygen							
Si	2.73	2.97	2.68	2.70	2.61	2.74	2.97
Al	1.27	1.04	1.32	1.31	1.41	1.27	1.05
Fe+++	0.00	0.00	0.00	0.00	0.00	0.01	0.00
sum	4.00	4.02	4.00	4.01	4.02	4.01	4.02
Ca	0.23	0.00	0.28	0.26	0.37	0.23	0.00
Na	0.79	0.18	0.75	0.73	0.59	0.75	0.17
K	0.01	0.81	0.01	0.01	0.01	0.01	0.81
sum	1.04	0.99	1.04	1.00	0.97	1.00	0.98
X(Ab)	0.76	0.18	0.72	0.73	0.61	0.75	0.17
X(Or)	0.01	0.82	0.01	0.01	0.01	0.01	0.83
X(An)	0.22	0.00	0.27	0.26	0.38	0.23	0.00

Table DR1 (cont). Electron microprobe analyses of plagioclase and potassium feldspar.

Samples	WL2A	WL2A	WL2B	WL3	LB1	LB1	LB2
	(Pl)	(Pl)*	(Pl)	(Pl)	(Pl)	(Ks)	(Pl)
SiO2	44.83	55.61	44.38	60.3	63.82	64.60	63.93
Al2O3	34.82	28.01	35.43	25.21	23.12	19.16	23.03
Fe2O3	0.09	0.06	0.24	0.02	0.14	0.06	0.08
CaO	18.71	10.22	18.83	5.56	3.60	0.00	3.19
Na2O	0.98	6.12	0.82	8.74	9.29	1.82	9.64
K2O	0.01	0.03	0.01	0.11	0.22	13.68	0.10
sum	99.44	100.05	99.71	99.94	100.19	99.32	99.97
Cations on the Basis of 8 Oxygen							
Si	2.08	2.50	2.06	2.68	2.81	2.98	2.82
Al	1.91	1.49	1.93	1.32	1.20	1.04	1.20
Fe+++	0.00	0.00	0.01	0.00	0.01	0.00	0.00
sum	3.99	3.99	4.00	4.01	4.02	4.02	4.02
Ca	0.93	0.49	0.93	0.27	0.17	0.00	0.15
Na	0.09	0.53	0.07	0.75	0.79	0.16	0.82
K	0.00	0.00	0.00	0.01	0.01	0.80	0.01
sum	1.02	1.03	1.01	1.03	0.98	0.97	0.98
X(Ab)	0.09	0.52	0.07	0.74	0.81	0.17	0.84
X(Or)	0.00	0.00	0.00	0.01	0.01	0.83	0.01
X(An)	0.91	0.48	0.93	0.26	0.17	0.00	0.15

*Plagioclase inclusion in garnet.

Table DR1 (cont.) Average electron microprobe analyses of ilmenite.

Sample	GP1	SC1	SC2	WL2A	WL2B	WL3
SiO2	0.02	0.00	0.03	0.01	0.01	0.03
TiO2	54.34	52.96	54.06	53.23	52.93	54.09
Fe2O3	0.00	0.00	0.00	0.53	0.38	0.00
Al2O3.	0.00	0.00	0.01	0.00	0.00	0.02
MgO	0.33	0.74	0.33	0.92	0.45	0.32
CaO	0.01	0.03	0.01	0.01	0.01	0.00
MnO	1.10	0.59	0.76	0.30	0.70	1.18
FeO	45.02	45.59	45.69	45.64	46.01	44.60
sum	100.82	99.91	100.88	100.64	100.49	100.23
		Cations on the Basis of 6 Oxygen				
Si	0.00	0.00	0.00	0.00	0.00	0.00
Ti	2.03	2.00	2.02	1.99	1.99	2.03
Fe3+	0.00	0.00	0.00	0.02	0.01	0.00
Al	0.00	0.00	0.00	0.00	0.00	0.00
Mg	0.03	0.06	0.02	0.07	0.03	0.02
Ca	0.00	0.00	0.00	0.00	0.00	0.00
Mn	0.05	0.03	0.03	0.01	0.03	0.05
Fe2+	1.87	1.92	1.90	1.90	1.93	1.86
sum	3.97	4.00	3.98	4.00	4.00	3.97

Table DR1 (cont.) Average electron microprobe analyses of staurolite, cordierite, hercynite, and gedrite from samples AJM-WL2A and AJM-WL2B.

Mineral	Staurolite			Cordierite	Hercynite		Gedrite
Sample	WL2A	WL2A*	WL2B	WL2A	WL2A	WL2B	WL2A
SiO2	26.75	26.50	26.65	49.28	0.02	0.03	40.82
TiO2	0.75	0.63	0.65	0.01	0.00	0.81	0.32
Al2O3	53.92	52.73	54.56	33.49	60.60	59.83	18.69
Cr2O3	-	-	-	-	0.02	0.02	-
Fe2O3	-	-	-	0.63	2.30	1.68	6.48
FeO	12.51	13.20	12.20	5.07	29.60	28.37	13.60
MnO	0.08	0.07	0.16	0.04	0.08	0.14	0.32
MgO	2.46	3.62	3.18	10.54	7.47	7.76	14.25
CaO	0.00	0.00	0.06	0.02	-	-	0.30
ZnO	-	-	-	-	0.43	0.84	-
Na2O	-	-	-	0.42	-	-	2.29
K2O	-	-	-	0.00	-	-	0.01
sum	96.47	96.75	97.46	99.50	100.52	99.48	97.08
Cations		Basis = 48		Basis=18	Basis = 4		Basis=24
Si	7.50	7.45	7.39	4.96	0.00	0.00	5.95
Ti	0.16	0.13	0.14	0.00	0.00	0.02	0.04
Al	17.81	17.47	17.83	3.97	1.96	1.95	3.21
Cr	-	-	-	-	0.00	0.00	-
Fe3+	-	-	-	0.05	0.05	0.04	0.71
Fe2+	2.93	3.10	2.83	0.43	0.68	0.66	1.66
Mn	0.02	0.02	0.04	0.00	0.00	0.00	0.04
Mg	1.03	1.52	1.32	1.58	0.31	0.32	3.09
Ca	0.00	0.00	0.02	0.00	-	-	0.05
Zn	-	-	-	-	0.07	0.02	-
Na	-	-	-	0.08	-	-	0.65
K	-	-	-	0.00	-	-	0.00
sum	29.44	29.69	29.56	11.07	3.07	3.01	15.39

*Staurolite inclusion in garnet.

Table DR1 (cont.)

micas (MPLB-132)-All Fe as FeO; cations expressed per 11 oxygens.

oxide or element	biot 2 core	biot2 core	biot2 rim	biot2 rim	biot1 core	biot1 rim	musc 2	musc 1
SiO_2	35.15	33.73	34.02	33.41	33.87	34.85	46.75	45.99
Al_2O_3	19.98	20.25	19.85	20.09	20.81	19.99	37.22	36.49
TiO_2	2.56	2.46	2.47	2.39	2.41	2.60	0.53	0.65
MgO	8.00	7.84	7.83	7.94	7.25	7.83	0.58	0.71
FeO	19.28	20.21	20.39	20.44	19.27	20.43	1.14	1.40
MnO	.25	.23	.24	.24	.24	.25	.00	.00
CaO	.00	.00	.00	.00	.00	.00	.00	.13
Na_2O	.16	.16	.13	.14	.11	.16	.61	.53
K_2O	9.81	9.66	9.68	9.60	8.98	9.76	10.68	10.11
Total	95.21	94.58	94.60	94.25	92.96	95.90	97.51	96.04
Cations on the Basis of 11 Oxygens								
Si	2.681	2.611	2.633	2.600	2.636	2.656	3.037	3.032
Aliv	1.319	1.389	1.367	1.400	1.364	1.344	.963	.968
Alvi	.478	.459	.444	.443	.545	.452	1.888	1.868
Ti	.147	.143	.144	.140	.141	.149	.026	.032
Mg	.910	.904	.903	.921	.841	.889	.056	.070
Fe^{2+}	1.230	1.308	1.320	1.330	1.254	1.302	.062	.077
Mn	.016	.015	.016	.016	.016	.016	.000	.000
Sum Oct	2.782	2.832	2.830	2.850	2.798	2.810	2.032	2.049
Ca	.000	.000	.000	.000	.000	.000	.000	.009
Na	.023	.024	.020	.021	.016	.024	.077	.068
K	.955	.954	.956	.953	.892	.949	.885	.850
Sum A	.978	.978	.976	.974	.908	.973	.962	.927
Fe/Fe+Mg	.575	.591	.594	.591	.599	.594	.525	.524
X(Ca)	.000	.000	.000	.000	.000	.000	.000	.010
X(Na)	.024	.025	.020	.022	.018	.025	.080	.073
X(K)	.976	.975	.980	.978	.982	.975	.920	.917

Table DR1 (cont.)

Garnet (MPLB-132)-All Fe as FeO; cations expressed per 12 oxygens.

oxide	rim2	rim1	core2	core1
SiO_2	36.99	37.00	36.68	36.79
Al_2O_3	20.97	20.70	21.07	21.30
TiO_2	.00	.07	.05	.00
Cr_2O_3	.02	.00	.03	.00
MgO	2.50	2.36	3.73	2.97
FeO	31.02	30.98	33.48	31.78
MnO	7.55	8.18	3.74	6.14
CaO	1.46	1.51	1.39	1.52
Total	100.51	100.79	100.16	100.50
Si	2.984	2.986	2.955	2.962
Al	1.994	1.970	2.00	2.022
Ti	.000	.004	.003	.000
Cr^{3+}	.001	.000	.002	.000
Mg	.301	.284	.448	.356
Fe^{2+}	2.093	2.091	2.256	2.140
Mn	.516	.559	.255	.419
Ca	.126	.131	.120	.131
Fe/Fe+Mg	.874	.880	.834	.857
Pyrope	.099	.093	.146	.117
Almandine	.689	.682	.733	.703
Spessartine	.170	.182	.083	.138
Grossular	.042	.043	.039	.043

Table DR1 (cont.)

biotite (MPLB-134)-All Fe as FeO; cations expressed per 11 oxygens.

	core1	rim1	core2	rim2
SiO_2	34.39	34.31	34.09	34.64
Al_2O_3	19.08	18.64	19.18	18.96
TiO_2	3.20	3.13	2.79	3.06
Cr_2O_3	.08	.06	.05	.07
MgO	6.44	6.24	6.54	6.50
FeO	22.04	21.00	22.26	22.46
MnO	.09	.06	.08	.09
CaO	.00	.08	.00	.00
Na_2O	.24	.17	.22	.21
K_2O	9.24	9.00	9.24	9.24
Total	94.80	92.69	94.46	95.22
Si	2.671	2.710	2.662	2.682
Aliv	1.329	1.290	1.338	1.318
Alvi	.418	.446	.428	.413
Ti	.187	.186	.164	.178
Cr^{3+}	.005	.004	.003	.004
Mg	.745	.734	.761	.750
Fe^{2+}	1.432	1.387	1.454	1.454
Mn	.006	.004	.005	.006
Sum Oct	2.793	2.761	2.815	2.805
Ca	.000	.007	.000	.000
Na	.036	.026	.034	.031
K	.916	.907	.921	.913
Sum A	.952	.940	.955	.944
Fe/Fe+Mg	.658	.654	.656	.660
X(Ca)	.000	.007	.000	.000
X(Na)	.038	.028	.036	.033
X(K)	.962	.965	.964	.967

Table DR1 (cont.)

plagioclase (MPLB-134)-All Fe as FeO; cations expressed per 8 oxygens.

	1	1	2	2
SiO_2	66.28	65.64	64.75	66.11
Al_2O_3	24.62	24.94	23.77	24.16
FeO	.06	.08	.03	.08
CaO	4.24	4.75	4.08	4.19
Na_2O	8.72	8.26	9.18	8.77
K_2O	.15	.09	.20	.11
Total	104.06	103.77	102.01	103.43
Si	2.802	2.784	2.800	2.811
Al	1.227	1.247	1.212	1.211
Fe^{2+}	.002	.003	.001	.003
Ca	.192	.216	.189	.191
Na	.715	.679	.770	.723
K	.008	.005	.011	.006
An	.210	.240	.195	.208
Ab	.781	.754	.794	.786
Or	.009	.006	.011	.007

ilmenite (MPLB-134)-All Fe as FeO; cations expressed per 6 oxygens.

	1	2
TiO_2	51.96	52.43
Cr_2O_3	.02	.02
MgO	.10	.16
FeO	44.23	44.65
MnO	.89	.53
Total	97.27	97.85
Ti	2.018	2.022
Cr^{3+}	.001	.001
Mg	.008	.012
Fe^{2+}	1.910	1.915
Mn	.039	.023
Fe/Fe+Mg	.996	.994

Table DR1 (cont.)

garnet (MPLB-134)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO_2	36.42	36.47	37.04	36.95
Al_2O_3	20.81	20.85	20.83	20.91
TiO_2	.00	.00	.02	.00
Cr_2O_3	.00	.03	.00	.02
MgO	2.96	3.43	2.42	2.35
FeO	35.65	36.25	35.26	35.33
MnO	1.98	1.19	2.98	3.16
CaO	.98	.64	.92	.81
Total	98.80	98.85	99.46	99.54
Si	2.981	2.978	3.012	3.006
Al	2.008	2.007	1.997	2.005
Ti	.000	.000	.001	.000
Cr^{3+}	.000	.002	.000	.001
Mg	.361	.417	.293	.285
Fe^{2+}	2.440	2.476	2.398	2.404
Mn	.137	.082	.205	.218
Ca	.086	.056	.080	.071
Fe/Fe+Mg	.871	.856	.891	.894
Pyrope	.119	.138	.098	.096
Almandine	.807	.817	.806	.807
Spessartine	.045	.027	.069	.073
Grossular	.028	.018	.027	.024

Table DR1 (cont.)

biotite (MPLB-135)-All Fe as FeO; cations expressed per 11 oxygens.

	biotite1	biotite2
SiO_2	34.28	34.42
Al_2O_3	18.58	18.49
TiO_2	2.87	2.97
Cr_2O_3	.10	.06
MgO	7.00	7.15
FeO	21.55	21.11
MnO	.08	.09
CaO	.04	.00
Na_2O	.24	.26
K_2O	9.12	9.28
Total	93.84	93.83
Si	2.686	2.693
Aliv	1.314	1.307
Alvi	.402	.398
Ti	.169	.175
Cr^{3+}	.006	.004
Mg	.818	.834
Fe^{2+}	1.412	1.381
Mn	.005	.006
Sum Oct	2.812	2.798
Ca	.003	.000
Na	.036	.039
K	.912	.926
Sum A	.951	.965
Fe/Fe+Mg	.633	.623
X(Ca)	.003	.000
X(Na)	.038	.040
X(K)	.959	.960

Table DR1 (cont.)

garnet (MPLB-135)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO_2	36.04	36.17	37.06	36.38
Al_2O_3	20.98	20.94	21.01	20.80
TiO_2	.00	.07	.03	.00
Cr_2O_3	.02	.02	.03	.02
MgO	3.36	3.18	2.39	2.40
FeO	36.78	36.12	36.04	35.95
MnO	1.27	1.69	2.69	2.77
CaO	.85	.91	1.04	.97
Total	99.29	99.09	100.29	99.29
Si	2.943	2.955	2.993	2.978
Al	2.020	2.017	2.000	2.007
Ti	.000	.004	.002	.000
Cr^{3+}	.001	.001	.002	.001
Mg	.409	.387	.288	.293
Fe^{2+}	2.512	2.468	2.434	2.461
Mn	.088	.117	.184	.192
Ca	.074	.080	.090	.085
Fe/Fe+Mg	.860	.864	.894	.894
Pyrope	.133	.127	.096	.097
Almandine	.815	.809	.812	.812
Spessartine	.029	.038	.061	.063
Grossular	.024	.026	.030	.028

Table DR1 (cont.)

plagioclase (MPLB-135)-All Fe as FeO; cations expressed per 8 oxygens.

	1	2
SiO_2	65.72	64.78
Al_2O_3	24.37	24.51
FeO	.06	.06
CaO	4.39	4.50
Na_2O	9.09	8.83
K_2O	.15	.16
Total	103.77	102.85
Si	2.793	2.780
Al	1.221	1.240
Fe^{2+}	.002	.002
Ca	.200	.207
Na	.749	.735
K	.008	.009
An	.209	.218
Ab	.783	.773
Or	.008	.009

Table DR1 (cont.)

ilmenite (MPLB-135)-All Fe as FeO; cations expressed per 6 oxygens.

TiO_2	52.88
MgO	.16
FeO	44.94
MnO	.81
Total	98.81
Ti	2.021
Mg	.012
Fe^{2+}	1.910
Mn	.035
Fe/Fe+Mg	.994

Table DR1 (cont.)

biotite (MPWL-8a)-All Fe as FeO; cations expressed per 11 oxygens.

	1	2
SiO_2	38.05	38.75
Al_2O_3	18.07	18.14
TiO_2	1.55	1.69
MgO	14.80	14.51
FeO	14.76	14.15
MnO	.02	.02
Na_2O	.80	.60
K_2O	8.08	8.42
Total	96.13	96.28
Si	2.777	2.813
Aliv	1.223	1.187
Alvi	.332	.365
Ti	.085	.092
Mg	1.610	1.570
Fe^{2+}	.901	.859
Mn	.001	.001
Sum Oct	2.929	2.887
Na	.113	.085
K	.752	.780
Sum A	.865	.865
Fe/Fe+Mg	.359	.354
X(Na)	.131	.098
X(K)	.869	.902

Table DR1 (cont.)

ilmenite (MPWL-8a)-All Fe as FeO; cations expressed per 6 oxygens.

TiO_2	52.01
Cr_2O_3	.03
MgO	.13
FeO	47.96
MnO	.63
Total	100.78
Ti	1.970
Cr^{3+}	.001
Mg	.010
Fe^{2+}	2.020
Mn	.027
Fe/Fe+Mg	.995

Table DR1 (cont.)

plagioclase (MPWL-8a)-All Fe as FeO; cations expressed per 8 oxygens.

SiO_2	57.53
Al_2O_3	27.76
FeO	.11
CaO	9.26
Na_2O	6.38
K_2O	.04
Total	101.07
Si	2.552
Al	1.452
Fe^{2+}	.004
Ca	.440
Na	.549
K	.002
An	.444
Ab	.554
Or	.002

Table DR1 (cont.)

garnet (MPWL-8a)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO_2	39.38	39.64	38.71	38.84
Al_2O_3	21.45	22.30	21.84	21.82
TiO_2	.05	.00	.03	.00
MgO	6.30	8.08	6.40	7.26
FeO	30.39	29.87	31.02	29.43
MnO	.29	.64	1.28	.69
CaO	3.68	2.01	2.21	2.57
Total	101.53	102.53	101.49	100.60
Si	3.034	3.002	2.997	3.006
Al	1.948	1.991	1.993	1.991
Ti	.003	.000	.002	.000
Mg	.723	.912	.738	.837
Fe^{2+}	1.958	1.892	2.008	1.905
Mn	.019	.041	.084	.045
Ca	.304	.163	.183	.213
Fe/Fe+Mg	.730	.675	.731	.695
Pyrope	.241	.303	.245	.279
Almandine	.652	.629	.666	.635
Spessartine	.006	.014	.028	.015
Grossular	.101	.054	.061	.071

Table DR1 (cont.)

biotite (MPAL-51)-All Fe as FeO; cations expressed per 11 oxygens.

	matrix1	matrix2	adjacent to garnet1	adjacent to garnet2
SiO_2	34.74	35.01	35.33	31.85
Al_2O_3	16.36	16.21	17.16	17.16
TiO_2	3.46	4.35	1.60	1.61
MgO	9.65	9.07	10.07	8.36
FeO	21.84	21.39	22.60	26.38
MnO	.12	.08	.09	.32
CaO	.04	.05	.02	.43
Na_2O	.08	.09	.05	.35
K_2O	9.33	9.43	9.64	5.99
Total	95.62	95.68	96.56	92.45
Si	2.682	2.695	2.705	2.577
Aliv	1.318	1.305	1.295	1.423
Alvi	.171	.166	.254	.214
Ti	.201	.252	.092	.098
Mg	1.110	1.040	1.149	1.008
Fe^{2+}	1.410	1.377	1.447	1.785
Mn	.008	.005	.006	.022
Sum Oct	2.900	2.840	2.948	3.127
Ca	.003	.004	.002	.037
Na	.012	.014	.007	.055
K	.919	.926	.942	.618
Sum A	.934	.944	.951	.710
Fe/Fe+Mg	.560	.570	.557	.639
X(Ca)	.003	.004	.002	.052
X(Na)	.013	.015	.007	.077
X(K)	.984	.981	.991	.870

Table DR1 (cont.)

plagioclase (MPAL-51)-All Fe as FeO; cations expressed per 8 oxygens.

SiO_2	53.91
Al_2O_3	29.42
FeO	.03
CaO	10.95
Na_2O	5.16
K_2O	.09
Total	99.62
Si	2.439
Al	1.569
Fe^{2+}	.001
Ca	.531
Na	.453
K	.005
An	.537
Ab	.458
Or	.005

Table DR1 (cont.)

garnet (MPAL-51)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO_2	38.18	38.13	37.43	37.35
Al_2O_3	21.13	21.21	21.56	21.85
TiO_2	.00	.08	.03	.00
MgO	2.41	2.12	3.11	3.12
FeO	28.82	27.06	30.55	30.20
MnO	2.14	2.82	1.35	1.73
CaO	9.22	10.39	7.49	7.30
Total	101.89	101.82	101.53	101.55
Si	2.991	2.985	2.946	2.937
Al	1.951	1.958	2.000	2.025
Ti	.000	.005	.002	.000
Mg	.281	.247	.365	.366
Fe^{2+}	1.888	1.772	2.011	1.986
Mn	.142	.187	.090	.115
Ca	.774	.872	.632	.615
Fe/Fe+Mg	.870	.878	.846	.844
Pyrope	.091	.080	.118	.119
Almandine	.612	.576	.649	.644
Spessartine	.046	.061	.029	.037
Grossular	.251	.283	.204	.200

Table DR1 (cont).

Biotite (MPAL-311). All Fe as FeO; cations expressed per 11 oxygens.

	core2	rim2	core1	rim1
SiO2	35.68	35.73	35.74	35.69
Al2O3	18.70	19.02	18.62	18.58
TiO2	2.40	2.53	2.58	2.62
Cr2O3	.05	.05	.05	.07
MgO	9.62	9.53	9.63	9.37
FeO	18.53	17.99	18.29	18.91
MnO	.08	.05	.08	.08
CaO	.04	.04	.00	.00
Na2O	.28	.34	.26	.27
K2O	9.10	9.06	9.25	9.31
Total	94.47	94.33	94.50	94.90
Si	2.724	2.722	2.726	2.721
Aliv	1.276	1.278	1.274	1.279
Alvi	.407	.430	.400	.391
Ti	.138	.145	.148	.150
Cr3+	.003	.003	.003	.004
Mg	1.095	1.082	1.095	1.065
Fe2+	1.183	1.146	1.167	1.206
Mn	.005	.003	.005	.005
Sum Oct	2.831	2.809	2.818	2.821
Ca	.003	.003	.000	.000
Na	.041	.050	.039	.040
K	.886	.881	.900	.906
Sum A	.930	.934	.939	.946
Fe/Fe+Mg	.519	.514	.516	.531
X(Ca)	.003	.003	.000	.000
X(Na)	.044	.054	.042	.042
X(K)	.953	.943	.958	.958

Table DR1 (cont).
Ilmenite (MPAL-311). All Fe as FeO; cations expressed per 6 oxygens.

TiO2	53.06
MgO	.05
FeO	45.84
MnO	1.17
Total	100.14
Ti	2.008
Mg	.004
Fe2+	1.929
Mn	.050
Fe/Fe+Mg	.998

Table DR1 (cont.)

Plagioclase (MPAL-311). All Fe as FeO; cations expressed per 8 oxygens.

	1	2
SiO2	60.16	60.47
Al2O3	27.11	27.28
FeO	.03	.03
CaO	7.96	7.84
Na2O	7.21	7.25
K2O	.11	.07
Total	102.57	103.01
Si	2.617	2.619
Al	1.390	1.393
Fe2+	.001	.001
Ca	.371	.364
Na	.608	.609
K	.006	.004
An	.377	.373
Ab	.617	.623
Or	.006	.004

Table DR1 (cont.)

Garnet (MPAL-311). All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO2	38.14	37.62	37.83	37.00
Al2O3	21.42	21.43	21.57	21.34
MgO	4.19	4.16	3.60	3.56
FeO	33.39	34.24	33.61	33.71
MnO	1.49	1.64	2.35	2.58
CaO	3.06	2.39	2.52	2.42
Total	101.69	101.51	101.47	100.61
Si	2.994	2.970	2.986	2.959
Al	1.982	1.995	2.007	2.012
Mg	.490	.489	.423	.424
Fe2+	2.192	2.261	2.219	2.255
Mn	.099	.110	.157	.175
Ca	.257	.202	.213	.207
Fe/Fe+Mg	.817	.822	.840	.842
Pyrope	.161	.160	.140	.139
Almandine	.722	.738	.737	.737
Spessartine	.033	.036	.052	.057
Grossular	.085	.066	.071	.068

Table DR1 (cont.)

Sillimanite (MP-AL311). All Fe as Fe2O3; cations expressed per 20 oxygens.

SiO2	36.21
Al2O3	64.16
Fe2O3	.459
Cr2O3	.02
Total	100.81
Si	3.885
Al	8.114
Fe3+	.037
Cr3+	.002

Table DR1 (cont.)

biotite (MPAL-312)-All Fe as FeO; cations expressed per 11 oxygens.

	core1	rim1	2	core3	rim3
SiO_2	38.07	37.07	35.72	35.59	35.75
Al_2O	20.84	19.58	18.55	18.66	18.31
TiO_2	2.29	2.13	2.35	2.44	2.21
Cr_2O_3	.15	.05	.05	.08	.10
MgO	7.30	8.30	9.49	9.27	9.42
FeO	15.50	17.10	19.18	18.75	18.51
MnO	.06	.05	.05	.05	.06
Na_2O	.15	.21	.24	.30	.26
K_2O	9.70	9.07	9.35	8.52	8.37
Total	94.08	93.59	94.97	93.76	93.08
Si	2.851	2.817	2.723	2.732	2.758
Aliv	1.149	1.183	1.277	1.268	1.242
Alvi	.691	.571	.390	.421	.423
Ti	.129	.122	.135	.141	.128
Cr^{3+}	.009	.003	.003	.005	.006
Mg	.815	.940	1.078	1.061	1.083
Fe^{2+}	.971	1.087	1.223	1.204	1.194
Mn	.004	.003	.003	.003	.004
Sum Oct	2.619	2.726	2.832	2.835	2.838
Na	.022	.031	.036	.044	.039
K	.927	.879	.909	.834	.824
Sum A	.950	.912	.945	.886	.871
Fe/Fe+Mg	.544	.536	.532	.532	.524
X(Na)	.023	.034	.038	.050	.045
X(K)	.976	.964	.962	.941	.946

Table DR1 (cont.)

ilmenite (MPAL-312)-All Fe as FeO; cations expressed per 6 oxygens.

TiO_2	53.92
MgO	.09
FeO	46.75
MnO	1.07
Total	101.85
Ti	2.005
Mg	.007
Fe^{2+}	1.933
Mn	.045
Fe/Fe+Mg	.996

Table DR1 (cont.)

plagioclase (MPAL-312)-All Fe as FeO; cations expressed per 8 oxygens.

SiO_2	61.04	59.65	60.38	60.66
Al_2O_3	26.17	26.78	26.03	26.19
FeO	.00	.00	.11	.11
CaO	7.66	7.91	7.37	6.97
Na_2O	7.43	7.22	7.43	7.73
K_2O	.09	.12	.07	.09
Total	102.39	101.69	101.38	101.75
Si	2.655	2.619	2.654	2.656
Al	1.342	1.386	1.349	1.352
Fe^{2+}	.000	.000	.004	.004
Ca	.357	.372	.347	.327
Na	.627	.615	.633	.656
K	.005	.007	.004	.005
An	.361	.374	.353	.331
Ab	.634	.619	.643	.664
Or	.005	.007	.004	.005

Table DR1 (cont.)

garnet (MPAL-312)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	rim1	core2	rim2	core3	rim3
SiO_2	37.67	37.01	37.59	37.28	37.98	37.68
Al_2O_3	21.54	21.27	21.54	21.78	21.85	21.77
TiO_2	.05	.03	.03	.03	.00	.00
Cr_2O_3	.02	.05	.02	.05	.00	.03
MgO	3.15	3.05	3.25	3.93	4.26	3.93
FeO	33.94	33.98	34.12	32.86	33.43	32.93
MnO	1.82	1.59	1.54	1.57	.98	1.53
CaO	3.23	2.96	2.67	3.68	3.11	3.45
Total	101.41	99.94	100.76	101.18	101.61	101.30
Si	2.982	2.977	2.991	2.947	2.977	2.969
Al	2.010	2.017	2.020	2.030	2.019	2.022
Ti	.003	.002	.002	.002	.000	.000
Cr^{3+}	.001	.003	.001	.003	.000	.002
Mg	.372	.366	.385	.463	.498	.461
Fe^{2+}	2.247	2.286	2.270	2.172	2.192	2.170
Mn	.122	.108	.104	.105	.065	.102
Ca	.274	.255	.228	.312	.261	.291
Fe/Fe+Mg	.858	.862	.855	.824	.815	.825
Pyrope	.123	.121	.129	.152	.165	.152
Almandine	.745	.758	.760	.712	.727	.718
Spessartine	.040	.036	.035	.034	.022	.034
Grossular	.091	.085	.076	.102	.087	.096

Table DR1 (cont.)

micas (MPHP-12)-All Fe as FeO; cations expressed per 11 oxygens.

	biotite1	biotite2	muscovite1	muscovite2
SiO_2	33.89	34.19	49.17	47.11
Al_2O_3	19.06	18.69	36.36	35.72
TiO_2	2.72	3.03	.62	.75
MgO	8.15	7.76	.59	.57
FeO	22.35	21.51	1.28	1.29
MnO	.18	.23	.00	.00
CaO	.06	.05	.00	.00
Na_2O	.25	.07	.34	.43
K_2O	9.60	9.29	7.04	9.40
Total	96.27	94.82	95.40	95.26
Si	2.606	2.652	3.174	3.104
Aliv	1.394	1.348	.826	.896
Alvi	.334	.361	1.941	1.879
Ti	.157	.177	.030	.037
Mg	.934	.897	.057	.056
Fe^{2+}	1.437	1.395	.069	.071
Mn	.012	.015	.000	.000
Sum Oct	2.874	2.845	2.097	2.043
Ca	.005	.004	.000	.000
Na	.038	.010	.042	.055
K	.942	.919	.580	.790
Sum A	.985	.933	.622	.845
Fe/Fe+Mg	.606	.609	.548	.559
X(Ca)	.005	.004	.000	.000
X(Na)	.039	.011	.068	.065
X(K)	.956	.985	.932	.935

Table DR1 (cont.)

plagioclase (MPHP-12)-All Fe as FeO; cations expressed per 8 oxygens.

	core1	2	rim1
SiO_2	58.40	62.00	61.87
Al_2O_3	27.29	24.09	24.24
FeO	.00	.00	.08
CaO	5.35	5.46	5.36
Na_2O	7.58	8.27	8.42
K_2O	.26	.25	.16
Total	98.91	100.07	100.18
Si	2.618	2.744	2.737
Al	1.442	1.257	1.264
Fe^{2+}	.000	.000	.003
Ca	.257	.259	.254
Na	.659	.710	.722
K	.015	.014	.009
An	.276	.263	.258
Ab	.708	.722	.733
Or	.016	.014	.009

Table DR1 (cont.)

garnet (MPHP-12)-All Fe as FeO; cations expressed per 12 oxygens.

	core1	core2	rim1	rim2
SiO_2	37.29	37.05	36.64	36.40
Al_2O_3	21.25	21.08	21.97	21.32
TiO_2	.03	.07	.00	.00
MgO	2.97	2.95	2.40	2.59
FeO	33.19	33.05	32.62	32.69
MnO	6.98	6.37	7.42	7.40
CaO	1.50	1.55	1.43	1.17
Total	103.23	102.11	102.49	101.50
Si	2.944	2.952	2.914	2.927
Al	1.978	1.980	2.060	2.021
Mg	.350	.350	.285	.310
Fe^{2+}	2.191	2.202	2.170	2.198
Mn	.467	.430	.500	.504
Ca	.127	.132	.122	.101
Fe/Fe+Mg	.862	.863	.884	.876
Pyrope	.112	.112	.093	.100
Almandine	.699	.707	.705	.706
Spessartine	.149	.138	.162	.162
Grossular	.041	.042	.040	.032

Table DR1 (cont.).-Metabasite Mineral Compositional Data

amphiboles-All Fe as FeO; cations expressed per 23 oxygens; act=actinolite; symp=symplectic edenitic hornblende; core and rim analyses are for matrix edenitic hornblende.

	act	symp	core1	rim 1	core2	rim2	core3	rim3	core4	rim4
SiO_2	53.76	45.68	44.24	43.95	43.08	43.75	43.45	45.02	41.93	44.55
Al_2O_3	1.96	9.41	11.59	11.74	12.12	11.43	12.21	10.34	11.96	10.45
TiO_2	.15	.55	.84	.82	.72	.54	.75	.88	.82	.89
Cr_2O_3	.09	.81	.21	.19	.27	.26	.25	.25	.29	.31
MgO	13.09	9.49	10.37	10.13	8.66	8.71	9.09	9.79	8.73	9.51
FeO	15.64	17.50	15.58	15.62	17.87	18.16	16.45	16.77	16.83	17.40
MnO	.39	.38	.28	.25	.48	.40	.40	.44	.43	.40
CaO	12.43	11.55	11.78	11.73	11.39	11.40	11.49	11.63	11.37	11.70
Na_2O	.02	.90	1.23	1.23	1.27	1.17	1.28	1.11	1.21	1.08
K_2O	.15	.68	.98	1.02	1.09	.90	.94	.81	1.04	.84
Total	97.68	96.95	97.11	96.68	96.96	96.71	96.30	97.04	94.62	97.12
Si	7.671	6.887	6.623	6.612	6.544	6.653	6.588	6.768	6.513	6.721
Aliv	.329	1.113	1.377	1.388	1.456	1.347	1.412	1.232	1.487	1.279
Alvi	0	.560	.669	.695	.715	.702	.770	.601	.703	.579
Ti	.016	.062	.095	.093	.082	.062	.085	.099	.096	.101
Cr^{3+}	.010	.096	.025	.023	.033	.031	.030	.030	.036	.037
Mg	2.784	2.133	2.313	2.272	1.961	1.975	2.054	2.193	2.021	2.138
Fe^{2+}	1.867	2.206	1.951	1.966	2.271	2.309	2.086	2.109	2.186	2.195
Mn	.047	.048	.036	.032	.062	.052	.051	.056	.057	.051
Sum Oct	4.724	5.105	5.089	5.081	5.124	5.131	5.076	5.088	5.099	5.101
Ca	1.901	1.866	1.889	1.888	1.854	1.857	1.866	1.873	1.893	1.892
Na(M4)	.375	.029	.022	.031	.022	.012	.058	.039	.008	.007
Na(A)	0	.235	.336	.329	.353	.332	.319	.285	.357	.308
K	.027	.131	.187	.196	.211	.174	.181	.156	.206	.161
Sum A	.027	.366	.523	.525	.564	.506	.500	.441	.563	.469
Fe/Fe+Mg	.401	.508	.458	.464	.537	.539	.504	.490	.520	.507

Table DR1 (cont.) Metabasite Mineral Compositional Data

plagioclase-All Fe as FeO; cations expressed per 8 oxygens; symp=symplectite; core and rim analyses are for matrix plagioclase.

	symp	symp	core1	rim1	core2	rim2	core3	core4	rim4
SiO_2	44.16	47.81	56.61	46.98	55.94	48.33	54.94	48.43	47.97
Al_2O_3	35.81	31.91	27.30	33.00	27.31	32.30	27.30	32.05	32.15
FeO	.31	.38	.03	.13	.03	.16	.05	.08	.18
CaO	18.26	15.85	10.11	16.98	10.66	16.25	10.85	16.01	16.23
Na_2O	1.05	2.11	5.35	1.62	5.15	2.00	4.80	2.06	2.06
K_2O	.02	.07	.12	.03	.12	.03	.10	.05	.03
Total	99.61	98.13	99.52	98.75	99.21	99.07	98.05	98.70	98.64
Si	2.047	2.230	2.549	2.182	2.533	2.231	2.518	2.242	2.226
Al	1.957	1.755	1.449	1.807	1.458	1.758	1.475	1.749	1.759
Fe^{2+}	.011	.015	.001	.005	.001	.006	.002	.003	.007
Ca	.906	.792	.488	.845	.517	.804	.533	.794	.807
Na	.094	.191	.467	.146	.452	.179	.427	.185	.185
K	.001	.004	.007	.002	.007	.002	.006	.003	.002
An	.905	.802	.507	.851	.530	.816	.552	.809	.812
Ab	.094	.194	.485	.147	.463	.182	.442	.188	.186
Or	.001	.004	.007	.002	.007	.002	.006	.003	.002

Table DR1 (cont.) Metabasite Mineral Compositional Data

garnet-All Fe as FeO; cations expressed per 12 oxygens; symp=symplectite.

	symp	symp	core1	core2	core3	core4	rim1	rim2	rim3	rim4
SiO_2	37.81	38.64	38.46	38.62	38.28	38.44	38.73	38.50	38.48	38.69
Al_2O_3	21.57	20.91	21.45	21.33	20.71	20.82	21.65	21.20	21.07	21.26
TiO_2	.07	.05	.12	.05	.10	.05	.12	.09	.03	.03
Cr_2O_3	.35	.27	.26	.24	.05	.31	.21	.26	.24	.23
MgO	2.32	2.36	2.34	2.48	2.32	1.91	2.42	2.84	2.18	2.54
FeO	21.22	21.78	20.95	21.07	22.04	21.07	21.72	21.55	22.24	21.48
MnO	2.75	2.69	2.40	2.34	2.41	2.25	2.03	1.83	3.03	2.03
CaO	13.89	13.40	14.98	14.67	13.84	15.1	14.16	14.03	13.29	14.05
Total	99.98	100.12	100.96	100.80	99.76	99.99	101.04	100.30	100.56	100.31
Si	2.972	3.031	2.988	3.003	3.019	3.020	3.002	3.006	3.014	3.019
Al	1.999	1.934	1.965	1.955	1.926	1.928	1.979	1.951	1.946	1.956
Ti	.004	.003	.007	.003	.006	.003	.007	.005	.002	.002
Cr^{3+}	.022	.017	.016	.015	.003	.019	.013	.016	.015	.014
Mg	.272	.276	.271	.287	.273	.224	.280	.331	.254	.295
Fe^{2+}	1.395	1.429	1.361	1.370	1.454	1.384	1.408	1.407	1.457	1.402
Mn	.183	.179	.158	.154	.161	.150	.133	.121	.201	.134
Ca	1.170	1.126	1.247	1.222	1.170	1.274	1.176	1.174	1.115	1.175
Fe/Fe+Mg	.837	.838	.834	.827	.842	.861	.834	.810	.852	.826
Pyrope	.090	.092	.089	.095	.089	.074	.093	.109	.084	.098
Almandine	.462	.475	.448	.452	.475	.456	.470	.464	.481	.466
Spessartine	.061	.059	.052	.051	.053	.049	.044	.040	.066	.045
Grossular	.387	.374	.411	.403	.383	.420	.392	.387	.368	.391

Table DR1 (cont.) Metabasite Mineral Compositional Data

clinopyroxene-All Fe as FeO; cations expressed per 6 oxygens.

	core1	rim1	core2	rim2	core3	core4	rim4
SiO_2	52.83	53.08	52.72	52.34	53.33	53.25	52.95
Al_2O_3	1.33	.95	1.88	1.89	.18	.48	.38
TiO_2	.07	.07	.14	.07	.00	.00	.00
Cr_2O_3	.10	.07	.17	.17	.10	.07	.17
MgO	12.24	12.34	11.84	11.58	11.92	12.28	11.91
FeO	9.58	9.64	9.89	10.34	9.97	9.51	9.82
MnO	.28	.35	.28	.34	.56	.47	.56
CaO	23.21	23.64	22.89	22.57	23.94	24.20	23.85
Na_2O	.18	.17	.30	.31	.05	.07	.08
Total	99.83	100.29	100.12	99.61	100.07	100.32	99.72
Si	1.984	1.989	1.975	1.974	2.008	1.996	1.999
Al	.059	.042	.083	.084	.008	.021	.017
Ti	.002	.002	.004	.002	.000	.000	.000
Cr^{3+}	.003	.002	.005	.005	.003	.002	.005
Mg	.685	.689	.661	.651	.669	.686	.670
Fe^{2+}	.301	.302	.310	.326	.314	.298	.310
Mn	.009	.011	.009	.011	.018	.015	.018
Ca	.934	.949	.919	.912	.966	.972	.965
Na	.013	.012	.022	.023	.004	.005	.006
Fe/Fe+Mg	.305	.305	.319	.334	.319	.303	.316

Table DR1 (cont.) Metabasite Mineral Compositional Data

sphene-All Fe as FeO; cations expressed per 20 oxygens.

SiO_2	30.85
Al_2O_3	2.52
TiO_2	33.74
MgO	.01
FeO	.41
MnO	.06
CaO	28.20
Total	95.87
Si	4.180
Al	.403
Ti	3.438
Mg	.002
Fe^{2+}	.047
Mn	.007
Ca	4.094

Table DR2 begins here.

Sample MP-AL196, Amphibolite, mineral rims

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 14.57 on Tue 23 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997).

Activities and their uncertainties

	py	gr	alm	tr	ts	parg	di
a	0.00242	0.0948	0.0987	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.26037	0.44826	0.54883	0.50797	0.05000

	hed	cats	an	ab	q	H2O
a	0.350	0.0630	0.860	0.280	1.00	1.00
sd(a)/a	0.10007	0.26339	0.05000	0.15552	0	

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 27cats = 10py + 11gr + 6an + 6H2O
5) 2py + 3ts + 12hed = 4gr + 4alm + 3tr
6) 10gr + 6alm + 3tr + 3ab = py + 3parg + 18hed + 12an

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	8.9	6.13	93.25	5.73	-0.07390	-12.559	11.551	10.583
5	8.3	3.67	-243.47	10.79	0.23835	-6.908	12.769	3.163
6	8.2	1.13	339.25	13.30	-0.78383	29.704	13.914	4.237

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.46, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	10.7	1.4	825	74	0.648	1.41

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	11.10	1.47	850	79	0.721	1.34	-0.85	0.29

gr	10.50	1.53	834	82	0.329	1.40	0.22	0.59
alm	10.29	1.18	824	61	0.634	1.16	1.13	0.04
tr	10.71	1.54	828	83	0.716	1.41	0.09	0.24
ts	10.67	1.32	816	72	0.633	1.34	-0.86	0.08
parg	10.62	1.28	811	70	0.637	1.29	-1.11	0.09
di	10.41	1.29	798	73	0.663	1.28	0.81	0.09
hed	10.22	1.13	823	58	0.632	1.11	-1.30	0.06
cats	10.97	1.58	838	80	0.719	1.38	-0.53	0.34
an	10.77	1.49	825	73	0.603	1.40	0.17	0.09
ab	10.65	1.37	821	73	0.645	1.38	0.34	0.01
q	10.66	1.39	825	74	0.648	1.41	0	0
H2O	10.66	1.39	825	74	0.648	1.41	0	0

T = 825°C, sd = 74,
P = 10.7 kbars, sd = 1.4, cor = 0.648, sigfit = 1.41

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Sample MP-AL196, mineral rims

H2O Excluded

Activities and their uncertainties

	py	gr	alm	tr	ts	parg	di
a	0.00242	0.0948	0.0987	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.26037	0.44826	0.54883	0.50797	0.05000

	hed	cats	an	ab	q
a	0.350	0.0630	0.860	0.280	1.00
sd(a)/a	0.10007	0.26339	0.05000	0.15552	0

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) cats + q = an
4) 2py + 3ts + 12hed = 4gr + 4alm + 3tr
5) 10gr + 6alm + 3tr + 3ab = py + 3parg + 18hed + 12an

Calculations for the independent set of reactions

P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	10.3	1.39	-16.75	0.24	-0.01912	1.410	2.614	0.268
4	8.3	3.67	-243.47	10.79	0.23835	-6.908	12.769	3.163
5	8.2	1.13	339.25	13.30	-0.78383	29.704	13.914	4.237

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.

e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.42, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.0	667	69	0.759	0.75

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.32	1.11	685	74	0.794	0.64	-0.63	0.19
gr	9.06	1.05	661	76	0.535	0.74	-0.11	0.52
alm	9.04	1.01	677	76	0.731	0.72	0.19	0.13
tr	9.17	1.04	673	69	0.762	0.66	0.53	0.07
ts	9.02	1.02	668	69	0.762	0.74	-0.11	0.03
parg	9.07	1.01	669	69	0.759	0.68	-0.50	0.02
di	9.01	1.01	667	69	0.761	0.74	0.07	0.00
hed	9.05	1.02	680	78	0.725	0.72	-0.22	0.18
cats	8.21	1.36	619	88	0.859	0.55	0.73	0.59
an	8.98	1.09	666	69	0.739	0.75	-0.04	0.09
ab	9.02	1.01	667	69	0.759	0.73	0.15	0.00
q	9.00	1.01	667	69	0.759	0.75	0	0

T = 667°C, sd = 69,
P = 9.0 kbars, sd = 1.0, cor = 0.759, sigfit = 0.75

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Sample MP-AL196, mineral rims

Activities and their uncertainties

	py	gr	alm	tr	ts	parg	di
a	0.00242	0.0948	0.0987	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.26037	0.44826	0.54883	0.50797	0.05000

	hed	cats	an	ab	q	H2O
a	0.350	0.0630	0.860	0.280	1.00	0.750
sd(a)/a	0.10007	0.26339	0.05000	0.15552	0	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 27cats = 10py + 11gr + 6an + 6H2O
5) 2py + 3ts + 12hed = 4gr + 4alm + 3tr
6) 10gr + 6alm + 3tr + 3ab = py + 3parg + 18hed + 12an

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	8.2	6.18	99.64	5.73	-0.09232	-12.465	11.551	10.583
5	8.3	3.67	-243.47	10.79	0.23835	-6.908	12.769	3.163
6	8.2	1.13	339.25	13.30	-0.78383	29.704	13.914	4.237

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.46, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	10.5	1.2	804	63	0.642	1.27

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	10.87	1.28	828	67	0.716	1.19	-0.84	0.29
gr	10.32	1.35	812	70	0.324	1.26	0.19	0.59
alm	10.12	1.04	803	52	0.630	1.05	1.01.	0.04
tr	10.53	1.35	809	71	0.710	1.27	0.16	0.24
ts	10.46	1.17	797	62	0.627	1.21	-0.75	0.08
parg	10.41	1.12	791	60	0.631	1.16	-1.02	0.09
di	10.24	1.14	782	63	0.657	1.16	0.70	0.10
hed	10.06	1.00	803	50	0.627	1.00	-1.16	0.06
cats	10.67	1.40	813	68	0.712	1.25	-0.39	0.33
an	10.55	1.31	804	63	0.597	1.26	0.14	0.09
ab	10.44	1.20	801	62	0.639	1.24	0.31	0.01
q	10.45	1.22	804	63	0.642	1.27	0	0
H2O	10.45	1.22	804	63	0.642	1.27	0.03	0.00

T = 804°C, sd = 63,
P = 10.5 kbars, sd = 1.2, cor = 0.642, sigfit = 1.27

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Sample MP-AL196, mineral rims

Hedenbergite Excluded

Activities and their uncertainties

	py	gr	tr	ts	parg	di
a	0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

cats	an	ab	q	H2O	
a	0.0630	0.860	0.280	1.00	1.00
sd(a)/a	0.26339	0.05000	0.15552	0	

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 27cats = 10py + 11gr + 6an + 6H2O
5) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions (for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	8.9	6.13	93.25	5.73	-0.07390	-12.559	11.551	10.583
5	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.5	1.0	820	52	0.574	0.37

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.39	1.21	814	60	0.690	0.35	0.18	0.37
gr	9.43	1.12	825	58	0.275	0.35	0.12	0.48
tr	9.69	1.09	832	58	0.640	0.27	0.39	0.23
ts	9.53	1.03	819	53	0.530	0.37	-0.07	0.13
parg	9.56	1.02	815	53	0.535	0.28	-0.41	0.12
di	9.52	1.02	823	57	0.513	0.36	-0.08	0.13
cats	9.46	1.21	818	57	0.670	0.37	0.08	0.39
an	9.52	1.11	820	52	0.532	0.37	0.00	0.09
ab	9.53	1.02	819	52	0.565	0.35	0.12	0.01
q	9.52	1.02	820	52	0.574	0.37	0	0
H2O	9.52	1.02	820	52	0.574	0.37	0	0

T = 820°C, sd = 52,
P = 9.5 kbars, sd = 1.0, cor = 0.574, sigfit = 0.37

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Sample MP-AL196, mineral rims

Hedenbergite Excluded

Activities and their uncertainties

	py	gr	tr	ts	parg	di
a	0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

	cats	an	ab	q	H2O
a	0.0630	0.860	0.280	1.00	0.750
sd(a)/a	0.26339	0.05000	0.15552	0	

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 27cats = 10py + 11gr + 6an + 6H2O
5) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	8.2	6.18	99.64	5.73	-0.09232	-12.465	11.551	10.583
5	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.4	1.0	799	49	0.570	0.37

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.37	1.18	795	57	0.688	0.36	0.10	0.37
gr	9.37	1.10	802	55	0.270	0.36	0.09	0.48
tr	9.61	1.06	810	55	0.636	0.26	0.41	0.23
ts	9.44	1.00	798	50	0.525	0.37	-0.06	0.13
parg	9.48	1.00	794	50	0.530	0.28	-0.40	0.12

di	9.43	1.00	802	54	0.507	0.36	-0.08	0.13
cats	9.32	1.18	794	54	0.665	0.35	0.17	0.39
an	9.43	1.08	799	49	0.527	0.37	-0.01	0.09
ab	9.44	1.00	798	49	0.561	0.35	0.12	0.01
q	9.44	1.00	799	49	0.570	0.37	0	0
H2O	9.44	1.00	799	49	0.570	0.37	-0.00	0.00

T = 799°C, sd = 49,
P = 9.4 kbars, sd = 1.0, cor = 0.570, sigfit = 0.37

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Sample MP-AL196, mineral rims

Hedenbergite Excluded

Activities and their uncertainties

	py	gr	tr	ts	parg	di
a	0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

	cats	an	ab	q	H2O
a	0.0630	0.860	0.280	1.00	0.500
sd(a)/a	0.26339	0.05000	0.15552	0	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	8.6	3.37	214.49	4.93	-0.00688	-20.715	-4.132	9.590
5	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.3	1.0	775	46	0.581	0.39

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.34	1.17	775	54	0.700	0.39	-0.00	0.38
gr	9.30	1.08	777	51	0.290	0.39	0.05	0.47
tr	9.52	1.05	787	52	0.643	0.27	0.44	0.22
ts	9.35	0.99	775	47	0.537	0.39	-0.05	0.12
parg	9.37	0.99	770	47	0.540	0.31	-0.39	0.13
di	9.34	0.98	778	51	0.520	0.39	-0.08	0.13
cats	9.16	1.16	769	51	0.671	0.35	0.28	0.38
an	9.33	1.07	775	46	0.538	0.39	-0.02	0.09
ab	9.35	0.98	774	46	0.571	0.38	0.12	0.01
q	9.34	0.98	775	46	0.581	0.39	0	0
H2O	9.34	0.98	775	46	0.580	0.39	-0.00	0.00

T = 775°C, sd = 46,
P = 9.3 kbars, sd = 1.0, cor = 0.581, sigfit = 0.39

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Sample MP-AL196, mineral rims

Hedenbergite Excluded

Activities and their uncertainties

	py	gr	tr	ts	parg	di
a	0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

	cats	an	ab	q	H2O
a	0.0630	0.860	0.280	1.00	0.250
sd(a)/a	0.26339	0.05000	0.15552	0	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	7.5	3.41	229.52	4.93	-0.05073	-20.484	-4.132	9.593
5	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.1	0.9	732	41	0.580	0.48

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.27	1.13	737	49	0.702	0.47	-0.17	0.39
gr	9.16	1.04	731	46	0.294	0.48	-0.02	0.46
tr	9.34	1.01	743	46	0.643	0.37	0.49	0.22
ts	9.15	0.95	731	42	0.537	0.48	-0.02	0.12
parg	9.18	0.95	727	43	0.540	0.42	-0.39	0.13
di	9.14	0.94	734	46	0.520	0.48	-0.08	0.12
cats	8.84	1.11	722	46	0.668	0.38	0.49	0.37
an	9.12	1.02	732	41	0.538	0.48	-0.03	0.09
ab	9.15	0.94	731	42	0.571	0.47	0.12	0.01
q	9.14	0.94	732	41	0.580	0.48	0	0
H2O	9.15	0.94	732	42	0.578	0.48	-0.01	0.01

T = 732°C, sd = 41,
P = 9.1 kbars, sd = 0.9, cor = 0.580, sigfit = 0.48

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Sample MP-AL196, mineral rims

Hedenbergite Excluded

Activities and their uncertainties

	py	gr	tr	ts	parg	di
a		0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a		0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

	cats	an	ab	q	H2O
a	0.0630	0.860	0.280	1.00	0.100
sd(a)/a	0.26339	0.05000	0.15552	0	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) 3di + 3cats = py + 2gr

4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions
(for x(CO2) = 0.9 and x(H2O) = 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	4.0	3.34	-50.26	0.95	0.07787	-2.576	-1.057	1.177
4	5.6	3.43	235.87	4.93	-0.10013	-20.381	-4.132	9.603
5	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT (for x(CO2) = 0.9 and x(H2O) = 0.1)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.9	0.9	672	37	0.573	0.67

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.15	1.06	683	43	0.697	0.61	-0.42	0.39
gr	8.94	0.98	668	41	0.289	0.66	-0.13	0.46
tr	9.06	0.94	683	41	0.636	0.57	0.56	0.21
ts	8.86	0.89	672	37	0.530	0.67	0.00	0.12
parg	8.89	0.89	668	38	0.532	0.63	-0.39	0.13
di	8.86	0.88	673	40	0.513	0.67	-0.07	0.12
cats	8.40	1.04	658	40	0.660	0.46	0.81	0.37
an	8.82	0.96	672	37	0.530	0.67	-0.06	0.09
ab	8.87	0.89	671	37	0.563	0.66	0.12	0.01
q	8.86	0.88	672	37	0.573	0.67	0	0
H2O	8.86	0.89	672	38	0.566	0.67	-0.04	0.03

T = 672°C, sd = 37,
P = 8.9 kbars, sd = 0.9, cor = 0.573, sigfit = 0.67

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Sample MP-AL196, mineral rims

Hedenbergite, H2O Excluded

Activities and their uncertainties

py gr tr ts parg di

a	0.00242	0.0948	0.0184	0.00190	0.0149	0.630
sd(a)/a	0.67456	0.26645	0.44826	0.54883	0.50797	0.05000

	cats	an	ab	q
a	0.0630	0.860	0.280	1.00
sd(a)/a	0.26339	0.05000	0.15552	0

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 2py + 4gr + 3ts + 12q = 3tr + 12an
3) cats + q = an
4) 4py + 8gr + 9ts + 6ab = 3tr + 6parg + 24an

Calculations for the independent set of reactions

P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	7.9	3.91	-27.37	7.13	0.15696	-5.510	-9.118	2.799
2	7.8	0.99	-27.37	6.95	-0.38394	21.720	26.476	2.799
3	10.3	1.39	-16.75	0.24	-0.01912	1.410	2.614	0.268
4	8.2	1.43	-51.92	21.43	-0.85262	38.683	66.135	7.045

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.5	1.2	805	167	0.622	0.45

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.40	1.20	829	204	0.329	0.43	0.12	0.52
gr	9.42	1.19	821	192	0.414	0.43	0.10	0.33
tr	9.60	1.19	807	167	0.608	0.31	0.40	0.08
ts	9.48	1.17	805	167	0.615	0.45	-0.06	0.03
parg	9.53	1.17	807	167	0.620	0.34	-0.40	0.02
di	9.46	1.16	809	169	0.614	0.44	-0.08	0.02
cats	9.09	1.98	756	273	0.865	0.42	0.15	0.89
an	9.46	1.26	805	168	0.610	0.45	-0.00	0.07
ab	9.48	1.16	806	167	0.622	0.43	0.12	0.00
q	9.46	1.16	805	167	0.622	0.45	0	0

T = 805°C, sd = 167,
P = 9.5 kbars, sd = 1.2, cor = 0.622, sigfit = 0.45

Sample MP-AL196, Garnet Amphibolite symplectite

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 23.14 on Thu 1 Apr,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	tr	ts	parg	gl
a	0.00204	0.0915	0.0984	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.26080	0.47145	0.54150	0.54507	1.28406

	di	hed	cats	q	an	ab	H2O
a	0.630	0.350	0.0630	1.00	0.880	0.250	1.00
sd(a)/a	0.05000	0.10007	0.26339	0	0.05000	0.16875	

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 2py + 3ts + 12hed = 4gr + 4alm + 3tr
6) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
7) 2alm + 3tr + 3parg + 9ab = 3py + 2gr + 6gl + 6hed

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840
3	3.3	3.37	-50.26	0.95	0.07787	-2.576	-1.297	1.189
4	9.5	3.37	193.77	4.93	0.04080	-21.022	-4.089	9.727
5	6.5	3.71	-243.47	10.79	0.23835	-6.908	11.072	3.199
6	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
7	9.0	3.20	-60.05	7.76	0.56636	-19.357	-35.996	8.456

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	10.7	1.4	827	70	0.658	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	11.24	1.40	858	74	0.727	1.25	-1.07	0.28
gr	10.71	1.50	827	77	0.359	1.35	-0.01	0.58
alm	10.32	1.18	824	60	0.647	1.15	1.12	0.04
tr	10.46	1.46	814	76	0.718	1.33	-0.49	0.22
ts	10.70	1.34	823	71	0.644	1.33	-0.44	0.07
parg	10.66	1.23	814	65	0.651	1.23	-1.28	0.06
gl	10.73	1.33	834	70	0.653	1.32	0.64	0.07
di	10.41	1.20	796	66	0.670	1.17	1.01	0.08
hed	10.25	1.14	824	57	0.646	1.10	-1.29	0.05
cats	11.09	1.54	843	75	0.729	1.31	-0.64	0.35
q	10.70	1.35	827	70	0.658	1.35	0	0
an	10.82	1.45	828	70	0.621	1.34	0.18	0.09
ab	10.69	1.34	824	71	0.653	1.34	0.23	0.02
H2O	10.70	1.35	827	70	0.658	1.35	0	0

T = 827°C, sd = 70,
P = 10.7 kbars, sd = 1.4, cor = 0.658, sigfit = 1.35

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Sample MP-AL196, Garnet Amphibolite symplectite

Activities and their uncertainties

	py	gr	tr	ts	parg	gl
a	0.00204	0.0915	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.47145	0.54150	0.54507	1.28406

	di	cats	q	an	ab	H2O
a	0.630	0.0630	1.00	0.880	0.250	1.00
sd(a)/a	0.05000	0.26339	0	0.05000	0.16875	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
6) 3tr + 3ts + 6parg + 18ab = 4py + 8gr + 12gl

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840
3	3.3	3.37	-50.26	0.95	0.07787	-2.576	-1.297	1.189
4	9.5	3.37	193.77	4.93	0.04080	-21.022	-4.089	9.727
5	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
6	8.6	2.66	-363.57	15.48	1.37107	-45.623	-60.919	16.560

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.6	1.0	818	51	0.596	0.66

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.57	1.22	819	59	0.706	0.66	-0.03	0.37
gr	9.67	1.13	812	56	0.318	0.65	-0.17	0.47
tr	9.45	1.10	812	57	0.654	0.65	-0.24	0.20
ts	9.51	1.04	821	52	0.556	0.64	0.33	0.12
parg	9.61	1.03	812	52	0.571	0.57	-0.68	0.08
gl	9.54	1.03	828	52	0.581	0.47	1.00	0.08
di	9.56	1.03	812	55	0.543	0.64	0.17	0.11
cats	9.56	1.23	818	57	0.691	0.66	-0.02	0.40
q	9.55	1.03	818	51	0.596	0.66	0	0
an	9.58	1.12	818	51	0.563	0.66	0.04	0.08
ab	9.55	1.03	819	52	0.579	0.66	-0.05	0.03
H2O	9.55	1.03	818	51	0.596	0.66	0	0

T = 818°C, sd = 51,
P = 9.6 kbars, sd = 1.0, cor = 0.596, sigfit = 0.66

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Sample MP-AL196, Garnet Amphibolite symplectite

Activities and their uncertainties

	py	gr	tr	ts	parg	gl
a	0.00204	0.0915	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.47145	0.54150	0.54507	1.28406

	di	cats	q	an	ab	H2O
a	0.630	0.0630	1.00	0.880	0.250	0.750
sd(a)/a	0.05000	0.26339	0	0.05000	0.16875	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q

3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
6) 3tr + 3ts + 6parg + 18ab = 4py + 8gr + 12gl

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840
3	3.3	3.37	-50.26	0.95	0.07787	-2.576	-1.297	1.189
4	9.1	3.38	200.16	4.93	0.02238	-20.928	-4.089	9.727
5	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
6	8.6	2.66	-363.57	15.48	1.37107	-45.623	-60.919	16.560

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.5	1.0	798	49	0.595	0.63

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.55	1.20	802	57	0.707	0.63	-0.11	0.37
gr	9.61	1.11	791	53	0.318	0.62	-0.19	0.47
tr	9.39	1.08	793	54	0.653	0.63	-0.20	0.20
ts	9.42	1.02	801	49	0.555	0.61	0.35	0.12
parg	9.52	1.02	792	49	0.570	0.54	-0.65	0.09
gl	9.46	1.01	807	50	0.580	0.46	0.94	0.08
di	9.48	1.01	792	53	0.542	0.62	0.17	0.11
cats	9.42	1.21	796	54	0.689	0.63	0.07	0.40
q	9.47	1.01	798	49	0.595	0.63	0	0
an	9.49	1.10	798	49	0.562	0.63	0.03	0.08
ab	9.47	1.01	798	49	0.578	0.63	-0.05	0.03
H2O	9.47	1.01	798	49	0.595	0.63	0.00	0.00

T = 798°C, sd = 49,
P = 9.5 kbars, sd = 1.0, cor = 0.595, sigfit = 0.63

****

Sample MP-AL196, Garnet Amphibolite symplectite

Activities and their uncertainties

	py	gr	tr	ts	parg	gl
a	0.00204	0.0915	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.47145	0.54150	0.54507	1.28406

	di	cats	q	an	ab	H2O
a	0.630	0.0630	1.00	0.880	0.250	0.500
sd(a)/a	0.05000	0.26339	0	0.05000	0.16875	

Independent set of reactions

1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
6) 3tr + 3ts + 6parg + 18ab = 4py + 8gr + 12gl

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840
3	3.3	3.37	-50.26	0.95	0.07787	-2.576	-1.297	1.189
4	8.6	3.42	214.49	4.93	-0.00688	-20.715	-4.089	9.729
5	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
6	8.6	2.66	-363.57	15.48	1.37107	-45.623	-60.919	16.560

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.4	1.0	775	46	0.602	0.62

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.53	1.19	782	54	0.715	0.60	-0.21	0.38
gr	9.52	1.09	769	50	0.332	0.60	-0.22	0.46
tr	9.32	1.06	772	50	0.658	0.61	-0.16	0.20

ts	9.33	1.01	779	46	0.563	0.58	0.37	0.12
parg	9.42	1.00	770	47	0.576	0.53	-0.63	0.09
gl	9.37	1.00	783	47	0.587	0.47	0.87	0.08
di	9.38	1.00	770	50	0.550	0.60	0.16	0.11
cats	9.26	1.19	771	51	0.692	0.61	0.17	0.39
q	9.38	1.00	775	46	0.602	0.62	0	0
an	9.39	1.08	775	46	0.569	0.62	0.01	0.08
ab	9.38	1.00	776	46	0.585	0.62	-0.03	0.03
H2O	9.38	1.00	775	46	0.601	0.62	0.00	0.00

T = 775°C, sd = 46,
P = 9.4 kbars, sd = 1.0, cor = 0.602, sigfit = 0.62

****

Sample MP-AL196, Garnet Amphibolite symplectite

Activities and their uncertainties

	py	gr	tr	ts	parg	gl
a	0.00204	0.0915	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.47145	0.54150	0.54507	1.28406

	di	cats	q	an	ab	H2O
a	0.630	0.0630	1.00	0.880	0.250	0.250
sd(a)/a	0.05000	0.26339	0	0.05000	0.16875	

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q
3) 3di + 3cats = py + 2gr
4) 6tr + 21cats = 10py + 11gr + 6q + 6H2O
5) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
6) 3tr + 3ts + 6parg + 18ab = 4py + 8gr + 12gl

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840
3	3.3	3.37	-50.26	0.95	0.07787	-2.576	-1.297	1.189
4	7.5	3.46	229.52	4.93	-0.05073	-20.484	-4.089	9.732
5	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
6	8.6	2.66	-363.57	15.48	1.37107	-45.623	-60.919	16.560

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :

large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.2	1.0	734	42	0.602	0.62

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.47	1.15	745	49	0.718	0.57	-0.38	0.39
gr	9.36	1.05	727	45	0.334	0.58	-0.27	0.46
tr	9.16	1.02	732	46	0.657	0.61	-0.08	0.20
ts	9.14	0.97	737	42	0.563	0.58	0.41	0.12
parg	9.23	0.96	729	42	0.576	0.54	-0.59	0.09
gl	9.17	0.96	739	42	0.587	0.51	0.74	0.08
di	9.19	0.96	730	45	0.550	0.60	0.14	0.11
cats	8.95	1.14	726	46	0.690	0.58	0.37	0.39
q	9.19	0.96	734	42	0.602	0.62	0	0
an	9.18	1.04	734	42	0.568	0.62	-0.01	0.08
ab	9.19	0.96	734	42	0.585	0.62	-0.01	0.03
H2O	9.19	0.96	734	42	0.599	0.62	-0.00	0.01

T = 734°C, sd = 42,
P = 9.2 kbars, sd = 1.0, cor = 0.602, sigfit = 0.62

****

Sample MP-AL196, Garnet Amphibolite symplectite

Activities and their uncertainties

py	gr	tr	ts	parg	gl
a	0.00204	0.0915	0.0129	0.00250	0.0113	0.000243
sd(a)/a	0.68619	0.27158	0.47145	0.54150	0.54507	1.28406

	di	cats	q	an	ab
a	0.630	0.0630	1.00	0.880	0.250
sd(a)/a	0.05000	0.26339	0	0.05000	0.16875

Independent set of reactions
1) 3ts + 12di = 2py + 4gr + 3tr
2) 3tr + 12an = 2py + 4gr + 3ts + 12q
3) an = cats + q
4) 12parg + 36q = 2py + 4gr + 3tr + 3ts + 6gl
5) 3tr + 3ts + 6parg + 18ab = 4py + 8gr + 12gl

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	3.96	-27.37	7.13	0.15696	-5.510	-11.486	2.840
2	8.2	1.00	27.37	6.95	0.38394	-21.720	-25.342	2.840

3	10.1	1.39	16.75	0.24	0.01912	-1.410	-2.637	0.268
4	10.6	4.95	-186.00	15.20	0.81265	-15.678	-49.129	10.481
5	8.6	2.66	-363.57	15.48	1.37107	-45.623	-60.919	16.560

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.3	1.1	752	138	0.657	0.71

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.43	1.20	723	153	0.440	0.66	-0.31	0.43
gr	9.38	1.18	731	148	0.497	0.67	-0.24	0.27
tr	9.25	1.17	754	138	0.628	0.70	-0.11	0.09
ts	9.19	1.16	749	138	0.657	0.66	0.40	0.03
parg	9.36	1.15	757	138	0.658	0.61	-0.61	0.01
gl	9.46	1.17	804	152	0.667	0.53	0.80	0.24
di	9.28	1.15	749	138	0.651	0.69	0.15	0.01
cats	8.72	1.80	694	201	0.848	0.67	0.28	0.79
q	9.27	1.15	752	138	0.657	0.71	0	0
an	9.27	1.25	752	139	0.655	0.71	-0.00	0.07
ab	9.27	1.15	753	139	0.652	0.71	-0.02	0.02

T = 752°C, sd = 138,
P = 9.3 kbars, sd = 1.1, cor = 0.657, sigfit = 0.71

Sample AJM-AL1

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 19.45 on Thu 18 Mar,1999

(thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	pa	cel	sill	q
a	0.313	0.712	0.744	0.419	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.10121	0.52947	0	0

	san	H2O
a	0.840	1.00
sd(a)/a	0.05000	

Independent set of reactions

1) 3an + mu = gr + 3sill + san + H2O
2) 3an + pa = gr + ab + 3sill + H2O
3) 7phl + 12sill = 3east + 5py + 4mu
4) 3east + 6q = phl + py + 2mu
5) phl + east + 6q = py + 2cel
6) naph + 2sill + q = py + pa
7) ann + 2sill + q = alm + mu
8) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.6	1.74	29.48	0.65	0.05056	-3.964	-6.517	0.948
2	5.6	1.71	28.64	0.66	0.04440	-4.042	-6.108	0.948
3	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
4	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
5	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
6	15.4	68.02	23.76	0.84	0.00639	-1.931	0.081	18.097
7	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
8	5.5	1.32	-8.19	0.96	-0.11257	6.980	9.472	1.265

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.45
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.6	2.0	691	50	0.959	1.54

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	5.59	2.03	691	52	0.961	1.54	-0.03	0.04
ann	5.08	2.09	678	53	0.965	1.49	-0.88	0.16
east	5.64	2.01	692	51	0.960	1.54	0.17	0.02
naph	5.59	1.98	691	50	0.959	1.54	-0.11	0.00
py	5.39	2.11	686	54	0.964	1.53	0.39	0.15
gr	5.47	2.40	688	60	0.971	1.54	0.13	0.36
alm	5.38	2.03	686	52	0.962	1.52	0.41	0.03
an	5.54	2.18	690	55	0.965	1.54	-0.06	0.09
ab	5.69	1.79	700	46	0.951	1.39	-1.08	0.09
mu	6.03	1.63	687	41	0.939	1.25	-1.89	0.37
pa	5.82	1.46	714	38	0.941	1.13	2.18	0.38
cel	5.91	1.94	698	49	0.960	1.47	-1.23	0.06
sill	5.60	1.98	691	50	0.959	1.54	0	0
q	5.60	1.98	691	50	0.959	1.54	0	0
san	5.55	1.75	682	45	0.950	1.36	1.18	0.10
H2O	5.60	1.98	691	50	0.959	1.54	0	0

T = 691°C, sd = 50,
P = 5.6 kbars, sd = 2.0, cor = 0.959, sigfit = 1.54

****

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	cel	sill	q
a	0.313	0.712	0.744	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.52947	0	0

	san	H2O
a	0.840	1.00
sd(a)/a	0.05000	

Independent set of reactions

1) 3an + mu = gr + 3sill + san + H2O
2) 7phl + 12sill = 3east + 5py + 4mu
3) 3east + 6q = phl + py + 2mu
4) phl + east + 6q = py + 2cel
5) ann + 2sill + q = alm + mu
6) naph + 6an = py + 2gr + ab + 3sill + H2O
7) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.6	1.74	29.48	0.65	0.05056	-3.964	-6.517	0.948
2	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
3	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
4	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
5	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
6	6.9	11.72	24.61	1.48	0.16677	-11.273	-12.665	18.195
7	12.1	39.55	132.61	1.75	-0.01439	-6.645	-5.416	36.206

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.0	1.4	734	39	0.929	0.63

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	6.05	1.40	736	40	0.932	0.62	0.13	0.04
ann	5.66	1.49	724	42	0.940	0.57	-0.54	0.17
east	6.11	1.39	738	40	0.932	0.60	0.34	0.03
naph	6.01	1.36	734	39	0.929	0.63	-0.10	0.00
py	6.07	1.48	737	43	0.940	0.63	-0.12	0.18
gr	5.84	1.65	730	45	0.947	0.62	0.16	0.36
alm	5.86	1.42	730	40	0.934	0.61	0.25	0.04
an	5.93	1.49	733	42	0.938	0.63	-0.08	0.09
ab	6.01	1.36	734	39	0.929	0.63	0.00	0.00
mu	5.97	1.37	738	42	0.821	0.62	0.14	0.71
cel	6.29	1.39	741	39	0.930	0.44	-1.10	0.06
sill	6.01	1.36	734	39	0.929	0.63	0	0

q	6.01	1.36	734	39	0.929	0.63	0	0
san	6.00	1.37	733	41	0.898	0.63	0.06	0.21
H2O	6.01	1.36	734	39	0.929	0.63	0	0

T = 734°C, sd = 39,
P = 6.0 kbars, sd = 1.4, cor = 0.929, sigfit = 0.63

****

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	cel	sill	q
a	0.313	0.712	0.744	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.52947	0	0

	san	H2O
a	0.840	0.750
sd(a)/a	0.05000	

Independent set of reactions
1) 3an + mu = gr + 3sill + san + H2O
2) 7phl + 12sill = 3east + 5py + 4mu
3) 3east + 6q = phl + py + 2mu
4) phl + east + 6q = py + 2cel
5) ann + 2sill + q = alm + mu
6) naph + 6an = py + 2gr + ab + 3sill + H2O
7) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.2	1.75	30.55	0.65	0.04749	-3.948	-6.517	0.948
2	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
3	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
4	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
5	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
6	6.8	11.73	25.68	1.48	0.16370	-11.257	-12.665	18.195
7	11.7	39.74	134.74	1.75	-0.02053	-6.614	-5.416	36.207

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :

a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.8	1.3	700	35	0.927	0.55

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	5.77	1.34	701	36	0.931	0.55	0.04	0.04
ann	5.50	1.42	693	38	0.939	0.51	-0.41	0.17
east	5.84	1.33	703	36	0.930	0.53	0.28	0.03
naph	5.76	1.30	700	35	0.927	0.55	-0.10	0.00
py	5.73	1.41	699	38	0.938	0.55	0.06	0.17
gr	5.67	1.58	698	41	0.946	0.55	0.09	0.36
alm	5.65	1.35	698	37	0.933	0.53	0.19	0.04
an	5.72	1.43	699	38	0.937	0.55	-0.04	0.09
ab	5.76	1.30	700	35	0.927	0.55	0.00	0.00
mu	5.72	1.31	704	38	0.818	0.54	0.16	0.70
cel	6.01	1.33	706	36	0.929	0.36	-1.01	0.06
sill	5.76	1.30	700	35	0.927	0.55	0	0
q	5.76	1.30	700	35	0.927	0.55	0	0
san	5.75	1.31	699	37	0.896	0.55	0.04	0.20
H2O	5.76	1.30	700	35	0.925	0.55	0.01	0.01

T = 700°C, sd = 35,
P = 5.8 kbars, sd = 1.3, cor = 0.927, sigfit = 0.55

****

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	cel	sill	q
a	0.313	0.712	0.744	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.52947	0	0

	san	H2O
a	0.840	0.500
sd(a)/a	0.05000	

Independent set of reactions
1) 3an + mu = gr + 3sill + san + H2O

2) 7phl + 12sill = 3east + 5py + 4mu
3) 3east + 6q = phl + py + 2mu
4) phl + east + 6q = py + 2cel
5) ann + 2sill + q = alm + mu
6) naph + 6an = py + 2gr + ab + 3sill + H2O
7) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.8	1.77	32.94	0.65	0.04261	-3.912	-6.517	0.948
2	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
3	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
4	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
5	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
6	6.7	11.77	28.07	1.48	0.15882	-11.222	-12.665	18.195
7	11.3	40.17	139.51	1.75	-0.03029	-6.543	-5.416	36.207

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.5	1.2	665	32	0.924	0.49

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	5.48	1.27	665	32	0.928	0.48	-0.06	0.04
ann	5.34	1.36	661	35	0.936	0.47	-0.27	0.17
east	5.56	1.26	667	32	0.927	0.47	0.21	0.02
naph	5.50	1.24	665	32	0.924	0.48	-0.10	0.00
py	5.37	1.33	662	34	0.935	0.47	0.25	0.17
gr	5.49	1.50	665	37	0.944	0.49	0.01	0.36
alm	5.43	1.29	664	33	0.930	0.48	0.13	0.04
an	5.50	1.36	665	34	0.934	0.49	-0.00	0.09
ab	5.50	1.24	665	32	0.924	0.49	0.00	0.00
mu	5.45	1.25	669	34	0.816	0.47	0.18	0.65
cel	5.72	1.27	670	32	0.926	0.31	-0.91	0.06
sill	5.50	1.24	665	32	0.924	0.49	0	0
q	5.50	1.24	665	32	0.924	0.49	0	0
san	5.50	1.24	665	34	0.893	0.49	0.02	0.19
H2O	5.50	1.24	665	32	0.911	0.49	0.01	0.08

T = 665°C, sd = 32,
P = 5.5 kbars, sd = 1.2, cor = 0.924, sigfit = 0.49

****

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	cel	sill	q
a	0.313	0.712	0.744	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.52947	0	0

	san	H2O
a	0.840	0.250
sd(a)/a	0.05000	

Independent set of reactions
1) 3an + mu = gr + 3sill + san + H2O
2) 7phl + 12sill = 3east + 5py + 4mu
3) 3east + 6q = phl + py + 2mu
4) phl + east + 6q = py + 2cel
5) ann + 2sill + q = alm + mu
6) naph + 6an = py + 2gr + ab + 3sill + H2O
7) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.7	1.79	35.44	0.65	0.03531	-3.874	-6.517	0.949
2	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
3	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
4	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
5	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
6	6.3	11.81	30.57	1.48	0.15152	-11.183	-12.665	18.195
7	10.2	40.64	144.53	1.75	-0.04490	-6.466	-5.416	36.207

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.

hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.0	1.1	606	27	0.917	0.47

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	4.96	1.18	604	28	0.922	0.45	-0.26	0.04
ann	5.04	1.25	606	30	0.931	0.47	-0.01	0.16
east	5.07	1.16	606	28	0.920	0.47	0.10	0.02
naph	5.04	1.15	606	27	0.917	0.47	-0.10	0.00
py	4.76	1.23	599	29	0.928	0.37	0.62	0.16
gr	5.17	1.39	608	32	0.939	0.46	-0.14	0.37
alm	5.04	1.19	606	28	0.923	0.47	0.00	0.04
an	5.10	1.26	607	29	0.929	0.47	0.07	0.09
ab	5.05	1.15	606	27	0.917	0.47	0.00	0.00
mu	5.00	1.16	609	29	0.814	0.45	0.20	0.57
cel	5.21	1.17	609	28	0.919	0.36	-0.73	0.06
sill	5.05	1.15	606	27	0.917	0.47	0	0
q	5.05	1.15	606	27	0.917	0.47	0	0
san	5.05	1.15	606	29	0.888	0.47	-0.01	0.16
H2O	5.05	1.15	606	29	0.884	0.47	-0.01	0.19

T = 606°C, sd = 27,
P = 5.0 kbars, sd = 1.1, cor = 0.917, sigfit = 0.47

****

an independent set of reactions has been calculated

Activities and their uncertainties

	phl	ann	east	naph	py	gr	alm
a	0.0181	0.0643	0.0347	0.000553	0.00143	4.00e-5	0.329
sd(a)/a	0.44941	0.32332	0.39725	18.08318	0.70863	0.83949	0.15000

	an	ab	mu	cel	sill	q
a	0.313	0.712	0.744	0.00367	1.00	1.00
sd(a)/a	0.14176	0.05000	0.10000	0.52947	0	0

	san
a	0.840
sd(a)/a	0.05000

Independent set of reactions
1) 7phl + 12sill = 3east + 5py + 4mu
2) 3east + 6q = phl + py + 2mu
3) phl + east + 6q = py + 2cel

4) ann + 2sill + q = alm + mu
5) gr + alm + mu = ann + 3an
6) naph + 3an + san = py + gr + ab + mu

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	8.7	5.40	170.64	11.07	0.00528	-6.904	-15.933	4.902
2	5.2	4.70	45.25	10.42	-0.02569	-3.172	-1.072	1.471
3	4.5	2.99	65.55	3.95	0.02811	-3.671	-10.391	1.408
4	5.1	1.50	-17.73	1.24	0.02011	-1.967	1.336	0.370
5	4.9	1.03	45.53	1.38	-0.13608	7.267	5.302	1.011
6	7.1	18.00	-4.87	1.04	0.11621	-7.310	-6.149	18.122

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.2	1.4	629	103	0.744	0.51

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
phl	5.08	1.56	617	115	0.790	0.50	-0.18	0.15
ann	5.21	1.43	635	111	0.646	0.50	-0.12	0.34
east	5.30	1.47	634	107	0.761	0.50	0.14	0.05
naph	5.23	1.42	629	103	0.744	0.51	-0.10	0.00
py	4.44	1.88	567	142	0.859	0.40	0.47	0.52
gr	5.29	1.55	628	104	0.643	0.51	-0.08	0.41
alm	5.22	1.42	631	106	0.709	0.51	0.05	0.07
an	5.25	1.48	629	104	0.698	0.51	0.04	0.11
ab	5.23	1.42	629	103	0.744	0.51	0.00	0.00
mu	5.17	1.43	630	104	0.730	0.49	0.19	0.03
cel	5.60	1.50	655	109	0.770	0.34	-0.80	0.14
sill	5.23	1.42	629	103	0.744	0.51	0	0
q	5.23	1.42	629	103	0.744	0.51	0	0
san	5.23	1.42	629	103	0.744	0.51	-0.00	0.00

T = 629°C, sd = 103,
P = 5.2 kbars, sd = 1.4, cor = 0.744, sigfit = 0.51

****

Sample AJM AL2

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.50 on Sat 20 Mar,1999

(thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	alm	phl	ann	east	sill	q
a	0.00263	0.508	0.0165	0.0654	0.0323	1.00	1.00
sd(a)/a	0.66869	0.15000	0.50008	0.33230	0.41802	0	0

	ilm	ru	H2O
a	1.00	1.00	1.00
sd(a)/a	0	0	

Independent set of reactions
1) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm
2) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm
3) 2py + alm + 3ann + 12ru = 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	10.8	4.92	-27.19	10.45	-0.05909	3.742	5.280	2.088
2	5.8	2.72	25.77	10.48	-0.06152	6.924	-1.215	2.152
3	8.7	3.08	-135.38	10.90	0.00901	6.061	10.442	2.092

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.96
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.3	1.2	702	125	0.828	0.58

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.06	1.83	679	196	0.926	0.56	0.09	0.54

alm	8.25	1.51	703	129	0.499	0.58	0.01	0.96
phl	8.07	1.32	680	136	0.853	0.41	-0.33	0.13
ann	8.32	1.48	708	154	0.884	0.58	-0.04	0.18
east	8.40	1.28	717	130	0.841	0.42	0.33	0.06
sill	8.26	1.23	702	125	0.828	0.58	0	0
q	8.26	1.23	702	125	0.828	0.58	0	0
ilm	8.26	1.23	702	125	0.828	0.58	0	0
ru	8.26	1.23	702	125	0.828	0.58	0	0

T = 702°C, sd = 125,
P = 8.3 kbars, sd = 1.2, cor = 0.828, sigfit = 0.58

****

Sample AJM-AL3

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 11.44 on Sat 20 Mar,1999

(thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a	0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	cel	an	ab	sill	q
a	0.749	0.376	0.00209	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.54643	0.11349	0.05000	0	0

	ru	ilm	H2O
a	1.00	1.00	1.00
sd(a)/a	0	0	

Independent set of reactions

1) pa + 3an = gr + ab + 3sill + H2O
2) 7phl + 12sill = 5py + 3east + 4mu
3) 3east + 6q = py + phl + 2mu
4) phl + east + 6q = py + 2cel
5) naph + 2sill + q = py + pa
6) ann + 2sill + q = alm + mu
7) phl + 3an = py + gr + mu
8) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.4	1.59	28.64	0.66	0.04440	-4.042	-5.138	0.878
2	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
3	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
4	3.8	3.08	65.55	3.95	0.02811	-3.671	-10.780	1.461
5	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968
6	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
7	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
8	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.

e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.45
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.1	0.7	695	23	0.789	0.84

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.05	0.75	694	24	0.797	0.83	0.25	0.05
gr	7.06	0.78	695	24	0.795	0.84	0.12	0.14
alm	6.86	1.09	690	29	0.865	0.83	0.22	0.72
phl	7.10	0.74	695	24	0.792	0.84	0.08	0.01
ann	7.08	0.73	694	23	0.789	0.83	0.29	0.01
east	7.13	0.74	696	23	0.791	0.82	0.41	0.01
naph	7.09	0.73	695	23	0.789	0.84	-0.07	0.00
mu	7.09	0.73	695	23	0.788	0.84	0.14	0.00
pa	7.07	0.76	693	35	0.701	0.84	-0.05	0.79
cel	7.23	0.74	699	23	0.791	0.48	-1.88	0.02
an	7.08	0.75	695	24	0.791	0.84	-0.05	0.03
ab	7.09	0.74	695	26	0.755	0.84	0.02	0.15
sill	7.09	0.73	695	23	0.789	0.84	0	0
q	7.09	0.73	695	23	0.789	0.84	0	0
ru	7.09	0.73	695	23	0.789	0.84	0	0
ilm	7.09	0.73	695	23	0.789	0.84	0	0
H2O	7.09	0.73	695	23	0.789	0.84	0	0

T = 695°C, sd = 23,
P = 7.1 kbars, sd = 0.7, cor = 0.789, sigfit = 0.84

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Sample AJM-AL3

Celadonite Excluced

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a	0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	an	ab	sill	q
a	0.749	0.376	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.11349	0.05000	0	0

	ru	ilm	H2O
a	1.00	1.00	1.00
sd(a)/a	0	0	

Independent set of reactions

1) pa + 3an = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) naph + 2sill + q = py + pa
5) ann + 2sill + q = alm + mu
6) phl + 3an = py + gr + mu
7) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.4	1.59	28.64	0.66	0.04440	-4.042	-5.138	0.878
2	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
3	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
4	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968
5	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
6	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
7	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.44, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.3	0.7	700	24	0.792	0.25

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.26	0.77	700	24	0.801	0.25	-0.01	0.06
gr	7.25	0.79	700	24	0.798	0.25	0.04	0.14
alm	7.25	1.12	700	30	0.869	0.25	0.00	0.73
phl	7.24	0.75	699	24	0.794	0.22	-0.22	0.01
ann	7.25	0.75	699	24	0.792	0.23	0.23	0.01
east	7.28	0.75	700	24	0.793	0.20	0.30	0.01
naph	7.26	0.75	700	24	0.792	0.25	-0.07	0.00
mu	7.26	0.75	700	24	0.792	0.24	-0.10	0.00

pa	7.26	0.78	700	36	0.709	0.25	0.01	0.79
an	7.25	0.77	700	24	0.794	0.25	-0.02	0.03
ab	7.26	0.75	700	26	0.759	0.25	-0.01	0.15
sill	7.26	0.75	700	24	0.792	0.25	0	0
q	7.26	0.75	700	24	0.792	0.25	0	0
ru	7.26	0.75	700	24	0.792	0.25	0	0
ilm	7.26	0.75	700	24	0.792	0.25	0	0
H2O	7.26	0.75	700	24	0.792	0.25	0	0

T = 700°C, sd = 24,
P = 7.3 kbars, sd = 0.7, cor = 0.792, sigfit = 0.25

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Sample AJM-AL3

Celadonite Excluded

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a	0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	an	ab	sill	q
a	0.749	0.376	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.11349	0.05000	0	0

	ru	ilm	H2O
a	1.00	1.00	0.750
sd(a)/a	0	0	

Independent set of reactions
1) pa + 3an = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) naph + 2sill + q = py + pa
5) ann + 2sill + q = alm + mu
6) phl + 3an = py + gr + mu
7) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.0	1.59	29.71	0.66	0.04133	-4.026	-5.138	0.878
2	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
3	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
4	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968

5	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
6	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
7	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.44, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.1	0.7	672	22	0.785	0.30

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.03	0.73	671	22	0.795	0.29	0.15	0.05
gr	7.07	0.76	672	22	0.791	0.30	-0.07	0.14
alm	7.06	1.08	672	28	0.866	0.30	-0.00	0.73
phl	7.03	0.72	671	22	0.787	0.26	-0.29	0.01
ann	7.04	0.72	671	22	0.786	0.25	0.38	0.01
east	7.08	0.72	672	22	0.787	0.27	0.26	0.01
naph	7.06	0.72	672	22	0.785	0.30	-0.07	0.00
mu	7.06	0.72	672	22	0.785	0.29	-0.12	0.00
pa	7.07	0.74	674	33	0.696	0.30	0.05	0.78
an	7.06	0.73	672	22	0.788	0.30	0.03	0.03
ab	7.06	0.72	672	24	0.751	0.30	-0.02	0.14
sill	7.06	0.71	672	22	0.785	0.30	0	0
q	7.06	0.71	672	22	0.785	0.30	0	0
ru	7.06	0.71	672	22	0.785	0.30	0	0
ilm	7.06	0.71	672	22	0.785	0.30	0	0
H2O	7.06	0.72	672	22	0.783	0.30	-0.01	0.01

T = 672°C, sd = 22,
P = 7.1 kbars, sd = 0.7, cor = 0.785, sigfit = 0.30

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Sample AJM-AL3

Celadonite Excluded

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a	0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	an	ab	sill	q
a	0.749	0.376	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.11349	0.05000	0	0

	ru	ilm	H2O
a	1.00	1.00	0.500
sd(a)/a	0	0	

Independent set of reactions

1) pa + 3an = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) naph + 2sill + q = py + pa
5) ann + 2sill + q = alm + mu
6) phl + 3an = py + gr + mu
7) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.6	1.61	32.10	0.66	0.03645	-3.990	-5.138	0.879
2	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
3	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
4	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968
5	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
6	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
7	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.44, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.9	0.7	643	20	0.778	0.39

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.81	0.70	642	21	0.788	0.37	0.31	0.05
gr	6.90	0.72	644	21	0.784	0.38	-0.19	0.14
alm	6.87	1.03	643	26	0.863	0.39	-0.01	0.73
phl	6.82	0.69	642	20	0.780	0.34	-0.36	0.01
ann	6.84	0.69	642	20	0.779	0.31	0.54	0.01
east	6.87	0.69	643	20	0.780	0.38	0.21	0.01
naph	6.85	0.68	643	20	0.778	0.39	-0.07	0.00
mu	6.86	0.68	643	20	0.778	0.38	-0.15	0.00
pa	6.88	0.70	646	30	0.685	0.39	0.10	0.74
an	6.87	0.70	643	21	0.781	0.39	0.08	0.03
ab	6.86	0.69	644	23	0.744	0.39	-0.04	0.14
sill	6.85	0.68	643	20	0.778	0.39	0	0
q	6.85	0.68	643	20	0.778	0.39	0	0
ru	6.85	0.68	643	20	0.778	0.39	0	0
ilm	6.85	0.68	643	20	0.778	0.39	0	0
H2O	6.86	0.69	643	21	0.762	0.39	-0.03	0.06

T = 643°C, sd = 20,
P = 6.9 kbars, sd = 0.7, cor = 0.778, sigfit = 0.39

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Sample AJM-AL3

Celadonite Excluded

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph	
a		0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a		0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	an	ab	sill	q
a	0.749	0.376	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.11349	0.05000	0	0

	ru	ilm	H2O
a	1.00	1.00	0.250
sd(a)/a	0	0	

Independent set of reactions
1) pa + 3an = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) naph + 2sill + q = py + pa
5) ann + 2sill + q = alm + mu

6) phl + 3an = py + gr + mu
7) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.6	1.62	34.60	0.66	0.02915	-3.952	-5.138	0.880
2	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
3	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
4	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968
5	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
6	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
7	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information
avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.44, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.5	0.6	591	18	0.762	0.63

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.41	0.65	589	18	0.772	0.56	0.62	0.05
gr	6.60	0.67	593	18	0.768	0.60	-0.44	0.14
alm	6.52	0.96	592	23	0.853	0.63	-0.02	0.73
phl	6.46	0.64	590	18	0.765	0.57	-0.51	0.01
ann	6.47	0.63	590	18	0.763	0.49	0.87	0.01
east	6.51	0.64	591	18	0.764	0.62	0.12	0.01
naph	6.50	0.63	591	18	0.762	0.63	-0.07	0.00
mu	6.51	0.63	591	18	0.762	0.61	-0.21	0.00
pa	6.54	0.65	597	26	0.667	0.61	0.18	0.66
an	6.54	0.65	592	18	0.765	0.61	0.19	0.03
ab	6.51	0.64	592	20	0.729	0.62	-0.08	0.12
sill	6.50	0.63	591	18	0.762	0.63	0	0
q	6.50	0.63	591	18	0.762	0.63	0	0
ru	6.50	0.63	591	18	0.762	0.63	0	0
ilm	6.50	0.63	591	18	0.762	0.63	0	0
H2O	6.51	0.64	593	20	0.723	0.62	-0.08	0.15

T = 591°C, sd = 18,
P = 6.5 kbars, sd = 0.6, cor = 0.762, sigfit = 0.63

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Sample AJM-AL3

Celadonite, Water Excluded

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00115	0.000190	0.400	0.0102	0.0724	0.0237	0.000323
sd(a)/a	0.72129	0.79949	0.15000	0.48518	0.30605	0.42949	30.95975

	mu	pa	an	ab	sill	q
a	0.749	0.376	0.385	0.663	1.00	1.00
sd(a)/a	0.10000	0.11666	0.11349	0.05000	0	0

	ru	ilm
a	1.00	1.00
sd(a)/a	0	0

Independent set of reactions

1) 7phl + 12sill = 5py + 3east + 4mu
2) 3east + 6q = py + phl + 2mu
3) naph + 2sill + q = py + pa
4) ann + 2sill + q = alm + mu
5) phl + 3an = py + gr + mu
6) alm + 2mu + 3ilm = 2ann + 3sill + 3ru

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	10.6	5.63	170.64	11.07	0.00528	-6.904	-14.090	5.134
2	6.0	4.86	45.25	10.42	-0.02569	-3.172	-0.708	1.567
3	16.2	116.39	23.76	0.84	0.00639	-1.931	0.293	30.968
4	5.4	1.45	-17.73	1.24	0.02011	-1.967	1.421	0.355
5	6.8	1.29	8.19	0.96	0.11257	-6.980	-8.171	1.233
6	4.3	2.51	35.71	2.49	-0.02011	2.156	-3.758	0.661

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.4	1.2	711	115	0.848	0.28

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.42	1.42	718	142	0.900	0.27	-0.07	0.38
gr	7.36	1.15	714	120	0.819	0.27	0.07	0.27
alm	7.34	1.39	711	115	0.748	0.28	0.01	0.73
phl	7.27	1.21	702	121	0.862	0.25	-0.20	0.08
ann	7.24	1.30	697	136	0.883	0.26	0.17	0.31
east	7.45	1.18	721	117	0.855	0.20	0.32	0.03
naph	7.35	1.15	711	115	0.848	0.27	-0.07	0.00
mu	7.34	1.16	709	116	0.849	0.27	-0.09	0.01
pa	7.35	1.15	711	115	0.848	0.28	0.00	0.00
an	7.36	1.15	713	117	0.837	0.28	-0.03	0.05
sill	7.35	1.15	711	115	0.848	0.28	0	0
q	7.35	1.15	711	115	0.848	0.28	0	0
ru	7.35	1.15	711	115	0.848	0.28	0	0
ilm	7.35	1.15	711	115	0.848	0.28	0	0

T = 711°C, sd = 115,
P = 7.4 kbars, sd = 1.2, cor = 0.848, sigfit = 0.28

MP-AL51

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.15 on Thu 25 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997).

An independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	gr	phl	ann	east	an
a	0.220	0.00350	0.0110	0.0390	0.0850	0.0250	0.690
sd(a)/a	0.15000	0.64745	0.54420	0.38642	0.28256	0.42526	0.05000

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 3alm + 2gr + 3east + 6q = 2py + 3ann + 6an
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	8.3	1.75	28.87	10.50	-0.25084	10.787	13.782	2.160
2	9.6	1.13	137.88	10.73	-0.44502	21.015	6.598	2.914
3	5.4	1.74	190.02	10.92	-0.32137	11.650	3.697	2.345
4	6.0	2.61	25.77	10.48	-0.06152	6.924	-1.422	2.027

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.9	3.0	566	226	0.818	3.09

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	8.21	2.49	605	174	0.801	2.33	-2.22	0.23
py	5.10	3.33	409	273	0.897	2.67	1.54	0.47
gr	6.43	2.25	660	186	0.676	2.33	2.26	0.62

phl	6.66	3.15	548	247	0.844	3.07	-0.40	0.11
ann	6.25	3.08	512	242	0.851	2.93	0.86	0.11
east	6.74	2.90	555	222	0.821	3.00	-0.86	0.01
an	6.80	2.88	579	223	0.797	3.00	-0.62	0.05
q	6.86	2.96	566	226	0.818	3.09	0	0
sill	6.86	2.96	566	226	0.818	3.09	0	0
ilm	8.61	3.04	646	204	0.841	2.55	1.76	0.32
ru	6.86	2.96	566	226	0.818	3.09	0	0

T = 566°C, sd = 226,
P = 6.9 kbars, sd = 3.0, cor = 0.818, sigfit = 3.09

****

MP-AL51

Activities and their uncertainties

	alm	py	phl	ann	east
a	0.220	0.00350	0.0390	0.0850	0.0250
sd(a)/a	0.15000	0.64745	0.38642	0.28256	0.42526

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm
2) 2alm + py + 3east + 6ru = 3phl + 6sill + 6ilm
3) alm + 2py + 3ann + 12ru = 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.0	2.61	25.77	10.48	-0.06152	6.924	-1.422	2.027
2	2.4	4.61	-27.19	10.45	-0.05909	3.742	9.772	1.890
3	10.6	3.09	-135.38	10.90	0.00901	6.061	8.663	2.099

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.96
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.3	1.6	843	166	0.667	1.06

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	6.38	1.91	840	172	0.369	1.06	-0.04	0.50
py	6.54	2.19	878	276	0.847	1.05	-0.09	0.63
phl	6.66	1.58	896	176	0.714	0.83	0.48	0.14
ann	6.17	1.71	824	194	0.739	1.04	0.11	0.15
east	6.13	1.50	821	159	0.675	0.70	-0.70	0.03
q	6.30	1.57	843	166	0.667	1.06	0	0
sill	6.30	1.57	843	166	0.667	1.06	0	0
ilm	6.26	2.17	843	166	0.524	1.06	-0.02	0.50
ru	6.30	1.57	843	166	0.667	1.06	0	0

T = 843°C, sd = 166,
P = 6.3 kbars, sd = 1.6, cor = 0.667, sigfit = 1.06

****

MP-AL51

Activities and their uncertainties

	py	gr	phl	ann	east	an
a	0.00350	0.0110	0.0390	0.0850	0.0250	0.690
sd(a)/a	0.64745	0.54420	0.38642	0.28256	0.42526	0.05000

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 3py + 4ann + 12ru = phl + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	8.3	1.75	28.87	10.50	-0.25084	10.787	13.782	2.160
2	9.6	1.13	137.88	10.73	-0.44502	21.015	6.598	2.914
3	12.5	3.89	-189.10	11.21	0.03252	5.773	12.025	2.681

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.30, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.96
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	10.2	1.6	659	96	0.867	0.68

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	10.52	2.60	679	156	0.948	0.66	-0.10	0.60
gr	10.23	1.84	658	102	0.585	0.68	-0.02	0.91
phl	10.50	1.80	678	107	0.890	0.53	0.30	0.12
ann	10.11	1.92	654	114	0.904	0.67	0.05	0.14
east	10.03	1.67	649	98	0.872	0.47	-0.41	0.03
an	10.20	1.65	659	97	0.842	0.68	0.01	0.07
q	10.20	1.64	659	96	0.867	0.68	0	0
sill	10.20	1.64	659	96	0.867	0.68	0	0
ilm	10.17	1.72	657	102	0.880	0.68	-0.03	0.04
ru	10.20	1.64	659	96	0.867	0.68	0	0

T = 659°C, sd = 96,
P = 10.2 kbars, sd = 1.6, cor = 0.867, sigfit = 0.68

Sample MP-AL311

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 15.24 on Tue 23 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	gr	phl	ann	east	an	a	0.520
sd(a)/a	0.15000	0.62553	0.75156	0.37927	0.37060	0.38400	0.06912		

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 3alm + 2gr + 3east + 6q = 2py + 3ann + 6an
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions (for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.6	1.85	28.87	10.50	-0.25084	10.787	16.313	2.333
2	6.4	1.33	137.88	10.73	-0.44502	21.015	16.041	3.569
3	5.7	1.87	190.02	10.92	-0.32137	11.650	3.275	2.600
4	6.7	2.53	25.77	10.48	-0.06152	6.924	-2.238	1.932

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a:
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.4	1.2	666	101	0.805	0.04

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	7.36	1.34	666	102	0.746	0.03	0.01	0.28
py	7.40	1.64	668	148	0.897	0.03	-0.01	0.48
gr	7.38	1.23	665	107	0.715	0.03	-0.02	0.46
phl	7.38	1.29	667	110	0.830	0.03	0.02	0.10
ann	7.37	1.44	666	127	0.865	0.04	-0.00	0.21
east	7.37	1.23	665	103	0.810	0.03	-0.02	0.02
an	7.37	1.22	666	102	0.789	0.03	0.01	0.03
q	7.37	1.22	666	101	0.805	0.04	0	0
sill	7.37	1.22	666	101	0.805	0.04	0	0
ilm	7.36	1.49	665	106	0.795	0.03	-0.01	0.34
ru	7.37	1.22	666	101	0.805	0.04	0	0

T = 666°C, sd = 101,
P = 7.4 kbars, sd = 1.2, cor = 0.805, sigfit = 0.04

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Sample MP-AL312

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 15.28 on Tue 23 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997).

an independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	gr	phl	ann	east	an
a	0.370	0.00513	0.00155	0.0410	0.0450	0.0370	0.490
sd(a)/a	0.15000	0.61633	0.70374	0.38162	0.37362	0.39138	0.07803

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.970	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) 3phl + 4sill = py + 3east + 4q
2) py + 2gr + 3east + 6q = 3phl + 6an
3) 3alm + 2gr + 3east + 6q = 2py + 3ann + 6an
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	19.6	88.20	26.71	10.43	0.01889	-0.186	-5.581	1.752
2	8.0	1.83	28.87	10.50	-0.25084	10.787	14.240	2.296
3	6.7	1.85	190.02	10.92	-0.32137	11.650	1.685	2.561
4	6.5	2.54	25.77	10.48	-0.06152	6.924	-1.967	1.947

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.4	1.1	627	91	0.804	0.88

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	7.87	1.26	632	91	0.754	0.68	-0.59	0.28
py	6.93	1.51	579	130	0.893	0.80	0.34	0.45
gr	7.31	1.15	658	97	0.706	0.59	0.80	0.47
phl	7.37	1.21	620	99	0.829	0.87	-0.13	0.11

ann	7.16	1.34	601	113	0.863	0.84	0.24	0.20
east	7.42	1.15	625	92	0.808	0.87	-0.12	0.02
an	7.41	1.14	634	92	0.781	0.83	-0.27	0.05
q	7.44	1.14	627	91	0.804	0.88	0	0
sill	7.44	1.14	627	91	0.804	0.88	0	0
ilm	8.02	1.41	648	96	0.803	0.73	0.49	0.34
ru	7.44	1.14	627	91	0.804	0.88	0	0

T = 627°C, sd = 91,
P = 7.4 kbars, sd = 1.1, cor = 0.804, sigfit = 0.88

Sample AJM-SC1

THERMOCALC v2.5, (c) Roger Powell and Tim Holland running at 11.22 on Sat 20 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

py	gr	alm	phl	ann	east	naph		
a		0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a		0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	1.00
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill
5) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	11.2	9.17	24.61	1.48	0.16677	-11.273	-6.029	14.246
4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
5	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	2.0	745	157	0.837	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.58	2.39	618	205	0.916	1.21	0.67	0.47
gr	8.75	1.45	807	122	0.768	0.95	1.44	0.39

alm	9.78	1.71	749	127	0.781	1.10	-1.01	0.29
phl	8.53	1.95	706	159	0.858	1.27	-0.65	0.11
ann	8.59	2.21	712	184	0.880	1.33	0.27	0.15
east	9.05	1.99	754	161	0.846	1.34	0.23	0.05
naph	8.95	1.95	745	157	0.837	1.35	-0.14	0.00
an	8.88	1.74	770	143	0.808	1.21	-0.69	0.09
ab	8.96	1.95	745	157	0.837	1.35	0.00	0.00
sill	8.96	1.95	745	157	0.837	1.35	0	0
q	8.96	1.95	745	157	0.837	1.35	0	0
ilm	10.20	1.99	789	138	0.824	1.14	0.88	0.35
ru	8.96	1.95	745	157	0.837	1.35	0	0
H2O	8.96	1.95	745	157	0.837	1.35	0	0

T = 745°C, sd = 157,
P = 9.0 kbars, sd = 2.0, cor = 0.837, sigfit = 1.35

****

Sample AJM-SC1

Grossular Excluded

Activities and their uncertainties

	py	alm	phl	ann	east	naph
a	0.00471	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.15000	0.45475	0.30527	0.40090	14.14427

	ab	sill	q	ilm	ru	H2O
a	0.675	1.00	1.00	0.959	1.00	1.00
sd(a)/a	0.05000	0	0	0.05000	0	

Independent set of reactions
1) alm + 3east + 4q = 2phl + ann + 4sill
2) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm
3) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm
4) 3east + naph + 12q + 9ilm = 3alm + 3phl + ab + 9ru + H2O

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
2	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969
3	4.4	2.67	25.77	10.48	-0.06152	6.924	0.310	2.102
4	8.5	17.90	54.20	10.48	-0.02376	-5.819	2.094	14.275

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.

hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.8	1.8	876	164	0.781	0.48

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.51	2.65	845	262	0.901	0.47	0.09	0.55
alm	8.77	2.07	878	171	0.538	0.48	0.02	0.50
phl	8.49	1.96	843	180	0.810	0.35	-0.37	0.13
ann	8.92	2.15	888	202	0.844	0.47	-0.06	0.18
east	9.02	1.89	899	171	0.794	0.33	0.41	0.06
naph	8.80	1.84	876	164	0.781	0.48	-0.09	0.00
ab	8.80	1.84	876	164	0.781	0.48	0.00	0.00
sill	8.80	1.84	876	164	0.781	0.48	0	0
q	8.80	1.84	876	164	0.781	0.48	0	0
ilm	8.83	2.38	877	165	0.645	0.48	0.01	0.50
ru	8.80	1.84	876	164	0.781	0.48	0	0
H2O	8.80	1.84	876	164	0.781	0.48	0	0

T = 876°C, sd = 164,
P = 8.8 kbars, sd = 1.8, cor = 0.781, sigfit = 0.48

****

Sample AJM-SC1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	0.750
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions
1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill
5) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	11.1	9.19	25.68	1.48	0.16370	-11.257	-6.029	14.246

4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
5	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.9	745	157	0.837	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.58	2.39	618	205	0.916	1.21	0.67	0.47
gr	8.75	1.45	807	122	0.768	0.95	1.44	0.39
alm	9.78	1.71	749	127	0.781	1.09	-1.01	0.29
phl	8.53	1.94	706	159	0.858	1.27	-0.66	0.11
ann	8.59	2.21	711	184	0.880	1.33	0.27	0.15
east	9.05	1.99	754	161	0.846	1.34	0.23	0.05
naph	8.95	1.95	745	157	0.837	1.35	-0.12	0.00
an	8.87	1.74	770	143	0.808	1.21	-0.69	0.09
ab	8.96	1.95	745	157	0.837	1.35	0.00	0.00
sill	8.96	1.95	745	157	0.837	1.35	0	0
q	8.96	1.95	745	157	0.837	1.35	0	0
ilm	10.20	1.99	789	138	0.824	1.14	0.88	0.35
ru	8.96	1.95	745	157	0.837	1.35	0	0
H2O	8.96	1.95	745	157	0.837	1.35	0.00	0.00

T = 745°C, sd = 157,
P = 9.0 kbars, sd = 1.9, cor = 0.837, sigfit = 1.35

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Sample AJM-SC1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	0.500
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill
5) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	11.0	9.22	28.07	1.48	0.15882	-11.222	-6.029	14.247
4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
5	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.9	745	157	0.837	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.58	2.39	618	205	0.916	1.21	0.67	0.47
gr	8.75	1.45	807	122	0.768	0.95	1.44	0.39
alm	9.78	1.71	749	127	0.781	1.09	-1.01	0.29
phl	8.53	1.94	706	159	0.858	1.27	-0.66	0.11
ann	8.59	2.20	711	184	0.880	1.33	0.27	0.15
east	9.05	1.99	754	161	0.846	1.34	0.23	0.05
naph	8.95	1.95	745	157	0.837	1.35	-0.11	0.00
an	8.87	1.74	770	143	0.808	1.21	-0.69	0.09
ab	8.96	1.95	745	157	0.837	1.35	0.00	0.00
sill	8.96	1.95	745	157	0.837	1.35	0	0
q	8.96	1.95	745	157	0.837	1.35	0	0
ilm	10.20	1.98	789	138	0.824	1.14	0.88	0.35
ru	8.96	1.95	745	157	0.837	1.35	0	0
H2O	8.96	1.95	745	157	0.837	1.35	0.00	0.00

T = 745°C, sd = 157,
P = 9.0 kbars, sd = 1.9, cor = 0.837, sigfit = 1.35

****

Sample AJM-SC1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	0.250
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill
5) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	10.6	9.25	30.57	1.48	0.15152	-11.183	-6.029	14.247
4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
5	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.9	745	157	0.837	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.57	2.38	618	205	0.916	1.21	0.67	0.47
gr	8.75	1.45	807	122	0.768	0.95	1.44	0.39
alm	9.78	1.71	748	127	0.781	1.09	-1.01	0.29
phl	8.53	1.94	705	159	0.857	1.26	-0.66	0.11
ann	8.58	2.20	711	184	0.880	1.32	0.27	0.15
east	9.05	1.99	753	161	0.846	1.34	0.23	0.05
naph	8.95	1.95	744	157	0.837	1.35	-0.07	0.00

an	8.87	1.74	770	143	0.808	1.21	-0.69	0.09
ab	8.95	1.95	745	157	0.837	1.35	0.00	0.00
sill	8.95	1.95	745	157	0.837	1.35	0	0
q	8.95	1.95	745	157	0.837	1.35	0	0
ilm	10.20	1.98	789	138	0.824	1.14	0.88	0.35
ru	8.95	1.95	745	157	0.837	1.35	0	0
H2O	8.95	1.95	745	157	0.837	1.35	0.00	0.00

T = 745°C, sd = 157,
P = 9.0 kbars, sd = 1.9, cor = 0.837, sigfit = 1.35

****

Sample AJM-SC1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	0.100
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions
1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill
5) py + 2alm + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(CO2) = 0.9 and x(H2O) = 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	10.1	9.26	31.63	1.48	0.14328	-11.166	-6.029	14.247
4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546
5	11.1	4.73	-27.19	10.45	-0.05909	3.742	5.095	1.969

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.9	744	157	0.837	1.35

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.57	2.38	618	204	0.916	1.21	0.67	0.47
gr	8.74	1.45	806	122	0.767	0.95	1.43	0.39
alm	9.77	1.70	748	127	0.781	1.09	-1.01	0.29
phl	8.52	1.94	705	159	0.857	1.26	-0.66	0.11
ann	8.58	2.20	710	183	0.880	1.32	0.27	0.15
east	9.04	1.98	753	161	0.846	1.34	0.23	0.05
naph	8.95	1.95	744	157	0.837	1.35	-0.01	0.00
an	8.87	1.74	769	143	0.808	1.20	-0.69	0.09
ab	8.95	1.94	744	157	0.837	1.35	0.00	0.00
sill	8.95	1.94	744	157	0.837	1.35	0	0
q	8.95	1.94	744	157	0.837	1.35	0	0
ilm	10.19	1.98	788	137	0.823	1.14	0.88	0.35
ru	8.95	1.94	744	157	0.837	1.35	0	0
H2O	8.95	1.94	744	157	0.837	1.35	0.00	0.00

T = 744°C, sd = 157,
P = 9.0 kbars, sd = 1.9, cor = 0.837, sigfit = 1.35

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Sample AJM-SC1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00471	0.00130	0.359	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.15000	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	H2O
a	0.383	0.675	1.00	1.00	1.00
sd(a)/a	0.11420	0.05000	0	0	

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) alm + 3east + 4q = 2phl + ann + 4sill

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	11.2	9.17	24.61	1.48	0.16677	-11.273	-6.029	14.246
4	16.0	32.38	27.00	10.48	-0.04240	0.474	0.430	1.546

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	13.6	3.3	907	180	0.892	0.48

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	13.11	4.81	875	286	0.951	0.47	0.09	0.54
gr	13.70	4.19	908	181	0.758	0.48	-0.02	0.81
alm	13.68	3.43	911	190	0.901	0.48	0.03	0.04
phl	13.00	3.53	869	197	0.907	0.35	-0.38	0.13
ann	13.84	3.84	921	220	0.922	0.48	-0.07	0.17
east	13.98	3.36	931	186	0.897	0.33	0.42	0.05
naph	13.61	3.28	907	180	0.892	0.48	-0.06	0.00
an	13.64	3.51	907	180	0.850	0.48	0.01	0.19
ab	13.62	3.28	907	180	0.892	0.48	0.00	0.00
sill	13.62	3.28	907	180	0.892	0.48	0	0
q	13.62	3.28	907	180	0.892	0.48	0	0
H2O	13.62	3.28	907	180	0.892	0.48	0	0

T = 907°C, sd = 180,
P = 13.6 kbars, sd = 3.3, cor = 0.892, sigfit = 0.48

****

Sample AJM-SC1

Activities and their uncertainties

	py	gr	phl	ann	east	naph
a	0.00471	0.00130	0.0167	0.0728	0.0333	0.000707
sd(a)/a	0.62356	0.71427	0.45475	0.30527	0.40090	14.14427

	an	ab	sill	q	ilm	ru	H2O
a	0.383	0.675	1.00	1.00	0.959	1.00	1.00
sd(a)/a	0.11420	0.05000	0	0	0.05000	0	

Independent set of reactions
1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) 3py + 4ann + 12ru = phl + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.9	1.38	137.88	10.73	-0.44502	21.015	11.773	3.706
2	10.3	1.94	28.87	10.50	-0.25084	10.787	10.826	2.491
3	11.2	9.17	24.61	1.48	0.16677	-11.273	-6.029	14.246
4	12.8	3.85	-189.10	11.21	0.03252	5.773	11.763	2.646

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.31, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	11.0	1.9	744	118	0.776	0.61

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	10.45	2.88	711	180	0.901	0.58	0.14	0.52
gr	10.91	2.26	746	129	0.404	0.60	0.02	0.81
phl	10.53	2.08	716	128	0.807	0.45	-0.46	0.12
ann	11.07	2.32	751	143	0.845	0.60	-0.05	0.17
east	11.28	2.01	764	122	0.793	0.44	0.48	0.06
naph	10.95	1.94	743	118	0.776	0.60	-0.15	0.00
an	10.95	2.01	744	120	0.673	0.60	-0.01	0.19
ab	10.96	1.94	744	118	0.776	0.61	0.00	0.00
sill	10.96	1.94	744	118	0.776	0.61	0	0
q	10.96	1.94	744	118	0.776	0.61	0	0
ilm	10.99	2.04	746	124	0.798	0.60	0.03	0.04
ru	10.96	1.94	744	118	0.776	0.61	0	0
H2O	10.96	1.94	744	118	0.776	0.61	0	0

T = 744°C, sd = 118,
P = 11.0 kbars, sd = 1.9, cor = 0.776, sigfit = 0.61

Sample AJM-SC2

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 17.07 on Sat 20 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00657	0.00283	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.66340	0.15000	0.39737	0.39641	0.36436	10.05025

	an	ab	ky	sill	q	ru	ilm
a	0.556	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05909	0.05820	0	0	0	0	0

	H2O
a	1.00
sd(a)/a	

Independent set of reactions

1) py + 3east + 4q = 3phl + 4ky
2) sill = ky
3) 4gr + 3phl + 12ky = py + 3east + 12an
4) naph + 6an = py + 2gr + ab + 3ky + H2O
5) 3alm + 3east + 4q = 2py + 3ann + 4ky
6) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
2	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
3	7.2	0.94	227.49	10.72	-0.59028	27.483	12.426	3.242
4	10.0	5.72	2.21	1.47	0.20309	-12.890	-6.908	10.161
5	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
6	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.7	1.0	638	47	0.990	1.30

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.53	1.07	630	49	0.991	1.27	0.46	0.12
gr	6.25	0.82	618	38	0.991	0.87	2.06	0.11
alm	7.75	1.18	686	54	0.995	1.09	-1.15	0.62
phl	6.60	1.01	634	47	0.990	1.26	-0.47	0.03
ann	6.62	1.07	634	49	0.991	1.29	0.20	0.07
east	6.72	1.01	639	47	0.990	1.29	0.25	0.01
naph	6.69	1.01	638	47	0.990	1.29	-0.32	0.00
an	6.60	0.96	634	45	0.990	1.22	-0.55	0.01
ab	6.69	1.01	638	47	0.990	1.30	0.00	0.00
ky	6.69	1.01	638	47	0.990	1.30	0	0
sill	6.69	1.01	638	47	0.990	1.30	0	0
q	6.69	1.01	638	47	0.990	1.30	0	0
ru	6.69	1.01	638	47	0.990	1.30	0	0
ilm	6.69	1.01	638	47	0.990	1.30	0	0
H2O	6.69	1.01	638	47	0.990	1.30	0	0

T = 638°C, sd = 47,
P = 6.7 kbars, sd = 1.0, cor = 0.990, sigfit = 1.30

****

Sample AJM-SC2

Grossular Excluded

Activities and their uncertainties

	py	alm	phl	ann	east	naph
a	0.00657	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.15000	0.39737	0.39641	0.36436	10.05025

	ab	ky	sill	q	ru	ilm
a	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05820	0	0	0	0	0

	H2O
a	1.00
sd(a)/a	

Independent set of reactions
1) py + 3east + 4q = 3phl + 4ky
2) sill = ky
3) 3alm + 3east + 4q = 2py + 3ann + 4ky
4) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru
5) 3alm + 3east + naph + 9ru = 3phl + ab + 6ky + 9ilm + H2O

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
2	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
3	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
4	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749
5	0.40	46.31	7.98	10.48	-0.07175	1.613	8.714	10.190

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.38, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.1	0.8	613	36	0.990	0.70

	P	sd(P)	T	sd(T)	cor	fit	e*·	hat
py	5.86	0.84	600	39	0.991	0.51	0.71	0.13
alm	6.69	1.15	638	53	0.995	0.59	-0.50	0.70
phl	6.01	0.80	607	37	0.990	0.57	-0.59	0.03
ann	5.98	0.83	606	38	0.991	0.63	0.40	0.07
east	6.15	0.78	614	36	0.990	0.69	0.18	0.01
naph	6.12	0.78	613	36	0.990	0.68	-0.33	0.00
ab	6.13	0.78	613	36	0.990	0.70	0.00	0.00
ky	6.13	0.78	613	36	0.990	0.70	0	0
sill	6.13	0.78	613	36	0.990	0.70	0	0
q	6.13	0.78	613	36	0.990	0.70	0	0
ru	6.13	0.78	613	36	0.990	0.70	0	0
ilm	6.13	0.78	613	36	0.990	0.70	0	0
H2O	6.13	0.78	613	36	0.990	0.70	0	0

T = 613°C, sd = 36,
P = 6.1 kbars, sd = 0.8, cor = 0.990, sigfit = 0.70

****

Sample AJM-SC2

Activities and their uncertainties

py	gr	alm	phl	ann	east	naph

a	0.00657	0.00283	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.66340	0.15000	0.39737	0.39641	0.36436	10.05025

	an	ab	ky	sill	q	ru	ilm
a	0.556	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05909	0.05820	0	0	0	0	0

	H2O
a	0.750
sd(a)/a	

Independent set of reactions

1) py + 3east + 4q = 3phl + 4ky
2) sill = ky
3) 4gr + 3phl + 12ky = py + 3east + 12an
4) naph + 6an = py + 2gr + ab + 3ky + H2O
5) 3alm + 3east + 4q = 2py + 3ann + 4ky
6) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
2	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
3	7.2	0.94	227.49	10.72	-0.59028	27.483	12.426	3.242
4	9.9	5.73	3.28	1.47	0.20002	-12.874	-6.908	10.161
5	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
6	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.7	1.0	638	47	0.990	1.29

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.53	1.07	630	49	0.991	1.27	0.46	0.12
gr	6.25	0.82	618	38	0.991	0.87	2.06	0.11
alm	7.75	1.18	686	54	0.995	1.09	-1.15	0.62

phl	6.60	1.01	634	47	0.990	1.26	-0.47	0.03
ann	6.62	1.07	634	49	0.991	1.29	0.20	0.07
east	6.72	1.01	639	47	0.990	1.28	0.25	0.01
naph	6.69	1.01	638	47	0.990	1.29	-0.29	0.00
an	6.60	0.96	634	44	0.990	1.22	-0.55	0.01
ab	6.69	1.01	638	47	0.990	1.29	0.00	0.00
ky	6.69	1.01	638	47	0.990	1.29	0	0
sill	6.69	1.01	638	47	0.990	1.29	0	0
q	6.69	1.01	638	47	0.990	1.29	0	0
ru	6.69	1.01	638	47	0.990	1.29	0	0
ilm	6.69	1.01	638	47	0.990	1.29	0	0
H2O	6.69	1.01	638	47	0.990	1.29	0.00	0.00

T = 638°C, sd = 47,
P = 6.7 kbars, sd = 1.0, cor = 0.990, sigfit = 1.29

****

Sample AJM-SC2

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00657	0.00283	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.66340	0.15000	0.39737	0.39641	0.36436	10.05025

	an	ab	ky	sill	q	ru	ilm
a	0.556	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05909	0.05820	0	0	0	0	0

	H2O
a	0.100
sd(a)/a	

Independent set of reactions
1) py + 3east + 4q = 3phl + 4ky
2) sill = ky
3) 4gr + 3phl + 12ky = py + 3east + 12an
4) naph + 6an = py + 2gr + ab + 3ky + H2O
5) 3alm + 3east + 4q = 2py + 3ann + 4ky
6) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions
(for x(CO2) = 0.9 and x(H2O) = 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
2	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
3	7.2	0.94	227.49	10.72	-0.59028	27.483	12.426	3.242
4	9.1	5.77	9.23	1.47	0.17960	-12.783	-6.908	10.162
5	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
6	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749

Average PT (for x(CO2) = 0.9 and x(H2O) = 0.1)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.7	1.0	638	47	0.990	1.29

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.52	1.06	630	49	0.991	1.26	0.45	0.12
gr	6.25	0.82	618	38	0.991	0.86	2.06	0.11
alm	7.74	1.17	686	54	0.995	1.08	-1.14	0.62
phl	6.60	1.00	633	46	0.990	1.25	-0.48	0.03
ann	6.61	1.06	634	49	0.991	1.28	0.21	0.07
east	6.71	1.01	639	47	0.990	1.28	0.25	0.01
naph	6.68	1.01	638	47	0.990	1.29	-0.14	0.00
an	6.59	0.96	634	44	0.990	1.21	-0.55	0.01
ab	6.69	1.01	638	47	0.990	1.29	0.00	0.00
ky	6.69	1.01	638	47	0.990	1.29	0	0
sill	6.69	1.01	638	47	0.990	1.29	0	0
q	6.69	1.01	638	47	0.990	1.29	0	0
ru	6.69	1.01	638	47	0.990	1.29	0	0
ilm	6.69	1.01	638	47	0.990	1.29	0	0
H2O	6.69	1.01	638	47	0.990	1.29	0.00	0.00

T = 638°C, sd = 47,
P = 6.7 kbars, sd = 1.0, cor = 0.990, sigfit = 1.29

****

Sample AJM-SC2

H2O Excluded

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00657	0.00283	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.66340	0.15000	0.39737	0.39641	0.36436	10.05025

	an	ab	ky	sill	q	ru	ilm
a	0.556	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05909	0.05820	0	0	0	0	0

Independent set of reactions

1) sill = ky
2) py + 3east + 4q = 3phl + 4ky
3) 4gr + 3phl + 12ky = py + 3east + 12an
4) 3alm + 3east + 4q = 2py + 3ann + 4ky
5) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
2	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
3	7.2	0.94	227.49	10.72	-0.59028	27.483	12.426	3.242
4	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
5	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.42, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.7	1.2	638	54	0.990	1.48

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.52	1.22	630	57	0.991	1.45	0.45	0.11
gr	6.24	0.82	618	38	0.991	0.99	2.06	0.11
alm	7.74	1.35	685	62	0.995	1.25	-1.14	0.62
phl	6.59	1.15	633	53	0.990	1.45	-0.48	0.03
ann	6.61	1.22	634	57	0.991	1.48	0.21	0.07
east	6.71	1.16	639	54	0.990	1.47	0.25	0.01
an	6.59	1.10	633	51	0.990	1.39	-0.55	0.01
ky	6.68	1.16	638	54	0.990	1.48	0	0
sill	6.68	1.16	638	54	0.990	1.48	0	0
q	6.68	1.16	638	54	0.990	1.48	0	0
ru	6.68	1.16	638	54	0.990	1.48	0	0
ilm	6.68	1.16	638	54	0.990	1.48	0	0

T = 638°C, sd = 54,
P = 6.7 kbars, sd = 1.2, cor = 0.990, sigfit = 1.48

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Sample AJM-SC2

Grossular, H2O Excluded

Activities and their uncertainties

	py	alm	phl	ann	east	naph
a	0.00657	0.322	0.0347	0.0380	0.0487	0.000995
sd(a)/a	0.59444	0.15000	0.39737	0.39641	0.36436	10.05025

	ab	ky	sill	q	ru	ilm
a	0.560	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.05820	0	0	0	0	0

Independent set of reactions

1) sill = ky
2) py + 3east + 4q = 3phl + 4ky
3) 3alm + 3east + 4q = 2py + 3ann + 4ky
4) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.9	0.11	-7.47	0.06	0.01211	-0.539	0	0
2	0.47	8.27	-56.58	10.43	0.02953	-1.969	4.004	1.723
3	13.2	16.67	104.57	10.85	-0.04100	-1.106	-7.390	2.055
4	8.9	4.39	27.19	10.45	0.05909	-3.742	-6.273	1.749

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.1	0.8	612	36	0.990	0.83

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.85	0.84	600	39	0.991	0.59	0.70	0.13
alm	6.67	1.15	637	53	0.995	0.69	-0.50	0.70
phl	6.00	0.80	607	37	0.990	0.65	-0.60	0.03
ann	5.97	0.83	605	38	0.991	0.73	0.41	0.07
east	6.14	0.78	613	36	0.990	0.81	0.17	0.01
ky	6.12	0.78	612	36	0.990	0.83	0	0

sill	6.12	0.78	612	36	0.990	0.83	0	0
q	6.12	0.78	612	36	0.990	0.83	0	0
ru	6.12	0.78	612	36	0.990	0.83	0	0
ilm	6.12	0.78	612	36	0.990	0.83	0	0

T = 612°C, sd = 36,
P = 6.1 kbars, sd = 0.8, cor = 0.990, sigfit = 0.83

Sample AJM-WL1

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 23.23 on Sat 20 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

	H2O
a	1.00
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions (for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655
2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	9.7	1.96	288.58	11.28	0.20752	-22.758	-34.189	5.941
4	15.2	42.79	132.61	1.75	-0.01439	-6.645	-2.487	39.172
5	9.1	1.29	51.29	2.53	0.02536	-6.561	-1.939	1.116
6	7.1	1.12	-83.51	10.76	0.56321	-28.498	-28.599	4.136

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.7	1.0	777	57	0.744	0.25

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.72	1.11	783	72	0.817	0.25	-0.11	0.40
gr	8.56	0.99	777	57	0.719	0.17	0.37	0.15
alm	8.81	1.32	780	59	0.702	0.24	-0.13	0.74
phl	8.66	0.99	778	59	0.759	0.25	0.05	0.06
ann	8.60	0.99	770	66	0.744	0.23	-0.18	0.34
east	8.66	0.98	778	59	0.756	0.25	0.04	0.06
naph	8.65	0.96	777	57	0.744	0.25	-0.10	0.00
an	8.60	0.98	777	57	0.731	0.22	-0.19	0.04
ab	8.65	0.96	777	57	0.744	0.25	0.00	0.00
san	8.65	0.97	777	59	0.748	0.25	0.02	0.02
q	8.65	0.96	777	57	0.744	0.25	0	0
sill	8.65	0.96	777	57	0.744	0.25	0	0
ru	8.65	0.96	777	57	0.744	0.25	0	0
ilm	8.65	0.96	777	57	0.744	0.25	0	0
H2O	8.65	0.96	777	57	0.744	0.25	0	0

T = 777°C, sd = 57,
P = 8.7 kbars, sd = 1.0, cor = 0.744, sigfit = 0.25

****

Sample AJM-WL1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

	H2O
a	0.750
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions (for X_{CO2}= 0.25 and X_{H2O}= 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655
2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	9.5	1.96	292.84	11.28	0.19524	-22.695	-34.189	5.941

4	14.8	42.99	134.74	1.75	-0.02053	-6.614	-2.487	39.172
5	8.6	1.30	53.42	2.53	0.01922	-6.529	-1.939	1.117
6	7.1	1.12	-83.51	10.76	0.56321	-28.498	-28.599	4.136

Average PT (for x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.4	0.9	742	51	0.709	0.18

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.32	1.00	739	64	0.786	0.18	0.06	0.38
gr	8.29	0.91	742	51	0.680	0.12	0.27	0.15
alm	8.54	1.24	745	53	0.679	0.15	-0.16	0.74
phl	8.35	0.90	741	53	0.726	0.18	-0.04	0.06
ann	8.36	0.90	742	60	0.705	0.18	0.01	0.34
east	8.35	0.90	742	53	0.722	0.18	-0.00	0.05
naph	8.35	0.88	742	51	0.709	0.18	-0.10	0.00
an	8.32	0.89	742	51	0.694	0.15	-0.14	0.04
ab	8.35	0.88	742	51	0.709	0.18	0.00	0.00
san	8.35	0.89	742	53	0.713	0.18	0.00	0.02
q	8.35	0.88	742	51	0.709	0.18	0	0
sill	8.35	0.88	742	51	0.709	0.18	0	0
ru	8.35	0.88	742	51	0.709	0.18	0	0
ilm	8.35	0.88	742	51	0.709	0.18	0	0
H2O	8.35	0.88	742	51	0.709	0.18	0.00	0.00

T = 742°C, sd = 51,
P = 8.4 kbars, sd = 0.9, cor = 0.709, sigfit = 0.18

****

Sample AJM-WL1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

	H2O
a	0.500
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions (for X_{CO2}= 0.5 and X_{H2O}= 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655
2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	9.2	1.98	302.39	11.28	0.17573	-22.553	-34.189	5.943
4	14.4	43.46	139.51	1.75	-0.03029	-6.543	-2.487	39.172
5	8.1	1.32	58.20	2.53	0.00946	-6.458	-1.939	1.119
6	7.1	1.12	-83.51	10.76	0.56321	-28.498	-28.599	4.136

Average PT (for x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.1	0.8	706	45	0.681	0.23

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.95	0.91	696	56	0.758	0.18	0.24	0.37
gr	8.03	0.84	706	45	0.650	0.21	0.15	0.15
alm	8.26	1.17	709	47	0.662	0.19	-0.18	0.74
phl	8.04	0.83	704	47	0.697	0.21	-0.12	0.06
ann	8.11	0.83	713	53	0.673	0.19	0.22	0.35
east	8.06	0.83	705	47	0.694	0.22	-0.05	0.05
naph	8.07	0.81	706	45	0.681	0.22	-0.10	0.00
an	8.05	0.83	706	45	0.664	0.22	-0.08	0.04
ab	8.07	0.81	706	45	0.681	0.23	0.00	0.00
san	8.07	0.82	706	47	0.684	0.23	-0.02	0.02
q	8.07	0.81	706	45	0.681	0.23	0	0
sill	8.07	0.81	706	45	0.681	0.23	0	0
ru	8.07	0.81	706	45	0.681	0.23	0	0
ilm	8.07	0.81	706	45	0.681	0.23	0	0

H2O	8.07	0.82	706	46	0.682	0.23	-0.01	0.01

T = 706°C, sd = 45,
P = 8.1 kbars, sd = 0.8, cor = 0.681, sigfit = 0.23

****

Sample AJM-WL1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

	H2O
a	0.250
sd(a)/a	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions (for X_{CO2}= 0.75 and X_{H2O}= 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655
2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	8.6	1.99	312.42	11.28	0.14650	-22.399	-34.189	5.945
4	13.4	43.97	144.53	1.75	-0.04490	-6.466	-2.487	39.172
5	7.0	1.34	63.21	2.53	-0.00515	-6.381	-1.939	1.122
6	7.1	1.12	-83.51	10.76	0.56321	-28.498	-28.599	4.136

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.6	0.7	644	38	0.641	0.49

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.36	0.80	626	47	0.719	0.35	0.58	0.35
gr	7.61	0.75	644	38	0.607	0.49	-0.09	0.15
alm	7.80	1.06	648	40	0.637	0.47	-0.20	0.74
phl	7.54	0.74	640	40	0.659	0.46	-0.29	0.06
ann	7.68	0.74	661	45	0.628	0.34	0.61	0.33
east	7.57	0.74	643	39	0.653	0.49	-0.12	0.04
naph	7.59	0.73	644	38	0.641	0.49	-0.10	0.00
an	7.60	0.74	644	38	0.623	0.49	0.05	0.04
ab	7.59	0.73	644	38	0.641	0.49	0.00	0.00
san	7.60	0.73	645	39	0.644	0.49	-0.06	0.02
q	7.59	0.73	644	38	0.641	0.49	0	0
sill	7.59	0.73	644	38	0.641	0.49	0	0
ru	7.59	0.73	644	38	0.641	0.49	0	0
ilm	7.59	0.73	644	38	0.641	0.49	0	0
H2O	7.60	0.73	645	39	0.644	0.49	-0.06	0.02

T = 644°C, sd = 38,
P = 7.6 kbars, sd = 0.7, cor = 0.641, sigfit = 0.49

Sample AJM-WL1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

	H2O
a	0.100
sd(a)/a	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) ann + 6an = 2gr + alm + san + 3sill + H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions (for X_{CO2}= 0.9 and X_{H2O}= 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655

2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	7.5	2.00	316.65	11.28	0.11356	-22.330	-34.189	5.953
4	11.6	44.21	146.64	1.75	-0.06137	-6.432	-2.487	39.172
5	6.4	1.20	-9.03	1.74	0.16316	-11.124	-8.642	1.830
6	7.1	1.12	-83.51	10.76	0.56321	-28.498	-28.599	4.136

Average PT (for x(H2O) = 0.1)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.0	0.6	566	32	0.599	0.97

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.65	0.70	538	39	0.679	0.72	1.07	0.34
gr	7.10	0.66	565	32	0.560	0.94	-0.47	0.15
alm	7.23	0.94	569	33	0.605	0.95	-0.23	0.74
phl	6.92	0.65	559	33	0.619	0.90	-0.55	0.06
ann	7.13	0.65	592	37	0.581	0.67	1.17	0.29
east	6.99	0.65	564	33	0.610	0.96	-0.23	0.04
naph	7.01	0.64	566	32	0.599	0.97	-0.10	0.00
an	7.06	0.65	566	32	0.578	0.95	0.24	0.04
ab	7.01	0.64	566	32	0.599	0.97	0.00	0.00
san	7.02	0.64	568	33	0.601	0.96	-0.11	0.02
q	7.01	0.64	566	32	0.599	0.97	0	0
sill	7.01	0.64	566	32	0.599	0.97	0	0
ru	7.01	0.64	566	32	0.599	0.97	0	0
ilm	7.01	0.64	566	32	0.599	0.97	0	0
H2O	7.05	0.65	571	35	0.608	0.95	-0.21	0.07

T = 566°C, sd = 32,
P = 7.0 kbars, sd = 0.6, cor = 0.599, sigfit = 0.97

****

Sample AJM-WL1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00272	0.000200	0.468	0.0197	0.0803	0.0258	0.000511
sd(a)/a	0.66627	0.79781	0.15000	0.44322	0.29092	0.42263	19.56947

	an	ab	san	q	sill	ru	ilm
a	0.322	0.699	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.13801	0.05000	0.05000	0	0	0	0

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 2gr + 3alm + 3east + 6q = 2py + 3ann + 6an
4) py + 3east + 12q + 12ilm = 4alm + 3phl + 12ru
5) py + 3east + 3ab + 12q + 12ilm = 4alm + 3naph + 3san + 12ru

Calculations for the independent set of reactions

P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	7.3	2.03	28.87	10.50	-0.25084	10.787	15.331	2.655
2	6.6	1.50	137.88	10.73	-0.44502	21.015	15.359	4.092
3	5.2	1.95	190.02	10.92	-0.32137	11.650	4.097	2.753
4	6.6	2.62	-25.77	10.48	0.06152	-6.924	2.064	2.044
5	1.1	71.86	13.41	10.77	0.05062	-5.934	-8.349	58.729

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.3	1.3	737	121	0.866	0.20

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.14	1.86	719	183	0.939	0.19	0.08	0.54
gr	8.34	1.27	747	127	0.843	0.13	0.25	0.25
alm	8.48	1.48	737	121	0.752	0.16	-0.16	0.75
phl	8.29	1.37	734	132	0.885	0.20	-0.05	0.12
ann	8.27	1.47	732	142	0.901	0.20	0.04	0.14
east	8.32	1.31	736	124	0.873	0.20	-0.01	0.04
naph	8.32	1.27	737	121	0.866	0.20	-0.10	0.00
an	8.33	1.27	742	124	0.854	0.17	-0.13	0.07
ab	8.32	1.27	737	121	0.866	0.20	0.00	0.00
san	8.32	1.27	737	121	0.866	0.20	-0.00	0.00
q	8.32	1.27	737	121	0.866	0.20	0	0
sill	8.32	1.27	737	121	0.866	0.20	0	0
ru	8.32	1.27	737	121	0.866	0.20	0	0
ilm	8.32	1.27	737	121	0.866	0.20	0	0

T = 737°C, sd = 121,
P = 8.3 kbars, sd = 1.3, cor = 0.866, sigfit = 0.20

Sample AJM-WL2A

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 22.58 on Mon 26 Apr,1999

(thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

An independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.0294	0.00145	0.249	0.106	0.0177	0.0623	0.0186
sd(a)/a	0.43031	0.70780	0.15000	0.27240	0.49188	0.33787	0.53856

	mst	fst	crd	fcrd	an	ab	sp
a	0.00482	0.294	0.621	0.0450	0.870	0.186	0.294
sd(a)/a	0.65106	0.20000	0.05000	0.37242	0.05000	0.19898	0.14950

	herc	ru	ilm	cor	sill	H2O
a	0.654	1.00	0.959	1.00	1.00	1.00
sd(a)/a	0.05000	0	0.05000	0	0	

Independent set of reactions

1) 5py + 2mst = 6crd + 11sp + 4H2O
2) 2mst + 5crd = 6py + 22sill + 4H2O
3) 2fst + 5fcrd = 6alm + 22sill + 4H2O
4) 6mst + 75an = 8py + 25gr + 96sill + 12H2O
5) 55gr + 6fst + 48fcrd = 40alm + 165an + 12H2O
6) py + 3herc = alm + 3sp
7) 60alm + 2fst + 110ru = 39fcrd + 110ilm + 4H2O
8) 5phl + 2crd + 6herc = 3py + 2alm + 5east
9) 3phl + 4cor = py + 3east
10) 7py + 19gr + 15phl + 6fst + 12ab = 8alm + 15east + 12naph + 57an
11) 2py + 3ann + 12an + 12ilm = 4gr + 7alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.9	0.50	241.16	4.30	-0.67752	44.782	11.986	3.020
2	7.8	1.19	311.55	3.93	-0.10663	-18.069	-8.110	2.902
3	6.0	0.77	111.90	2.67	-0.02979	-20.141	9.605	2.107
4	5.6	1.25	84.62	18.93	1.85099	-110.367	-149.191	18.822
5	5.3	5.92	699.35	38.64	-4.31965	54.427	437.113	44.051
6	17.5	46.14	-6.14	0.74	0.01131	-0.105	-0.260	0.657
7	5.4	0.47	1656.51	17.47	-3.63153	280.596	-39.630	17.955
8	5.0	1.76	29.25	17.42	0.17122	-14.443	-12.538	2.562
9	8.6	32.45	25.30	10.43	0.00931	0.444	-5.134	1.371
10	6.2	1.06	564.45	54.45	-2.39287	127.725	101.517	17.052
11	4.9	0.99	-244.66	11.17	0.63374	-29.361	-22.886	3.713

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.

e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.55, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.37
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.4	0.4	673	19	0.831	1.18

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.41	0.47	673	20	0.859	1.18	-0.03	0.30
gr	6.41	0.42	673	19	0.831	1.18	-0.28	0.04
alm	6.52	0.44	678	19	0.856	1.16	-0.72	0.17
phl	6.40	0.42	673	19	0.830	1.18	-0.06	0.02
ann	6.42	0.42	673	18	0.827	1.18	0.37	0.04
east	6.40	0.41	673	18	0.831	1.18	-0.18	0.00
naph	6.44	0.38	672	17	0.826	1.09	-1.46	0.04
mst	6.37	0.43	672	19	0.818	1.18	0.27	0.16
fst	6.54	0.43	687	24	0.821	1.14	0.64	0.52
crd	6.40	0.45	673	19	0.837	1.18	-0.02	0.06
fcrd	6.39	0.42	673	18	0.823	1.18	-0.22	0.08
an	6.40	0.42	673	19	0.831	1.18	0.06	0.00
ab	6.42	0.40	673	18	0.829	1.15	0.54	0.01
sp	6.25	0.41	667	18	0.845	1.10	1.37	0.13
herc	6.40	0.35	667	16	0.817	1.01	1.76	0.10
ru	6.40	0.41	673	19	0.831	1.18	0	0
ilm	6.36	0.36	674	16	0.826	1.03	-1.73	0.03
cor	6.40	0.41	673	19	0.831	1.18	0	0
sill	6.40	0.41	673	19	0.831	1.18	0	0
H2O	6.40	0.41	673	19	0.831	1.18	0	0

T = 673°C, sd = 19,
P = 6.4 kbars, sd = 0.4, cor = 0.831, sigfit = 1.18

****

Sample AJM-WL2A

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.0294	0.00145	0.249	0.106	0.0177	0.0623	0.0186
sd(a)/a	0.43031	0.70780	0.15000	0.27240	0.49188	0.33787	0.53856

	mst	fst	crd	fcrd	an	ab	sp
a	0.00482	0.294	0.621	0.0450	0.870	0.186	0.294
sd(a)/a	0.65106	0.20000	0.05000	0.37242	0.05000	0.19898	0.14950

	herc	ru	ilm	cor	sill	H2O
a	0.654	1.00	0.959	1.00	1.00	0.750
sd(a)/a	0.05000	0	0.05000	0	0	

Independent set of reactions
1) 6mst + 75an = 8py + 25gr + 96sill + 12H2O
2) 2mst + 45an = 15gr + 4crd + 40sill + 4H2O

3) 6fst + 75an = 25gr + 8alm + 96sill + 12H2O
4) 2fst + 45an = 15gr + 4fcrd + 40sill + 4H2O
5) py + 3herc = alm + 3sp
6) 20py + 9fst + 40cor = 9mst + 12crd + 36herc
7) 60alm + 2fst + 110ru = 39fcrd + 110ilm + 4H2O
8) 5phl + 2crd + 6herc = 3py + 2alm + 5east
9) 3phl + 3an + 3herc = py + gr + alm + 3east
10) 7py + 19gr + 15phl + 6fst - 12ab = 8alm + 15east + 12naph + 57an
11) 2py + 3ann + 12an + 12ilm = 4gr + 7alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.4	1.25	97.39	18.93	1.81415	-110.179	-149.191	18.823
2	5.3	1.55	-194.21	10.13	1.18352	-51.702	-83.026	10.933
3	5.4	1.18	183.18	16.93	1.79663	-112.439	-156.773	18.168
4	5.5	1.56	16.98	9.76	1.11154	-51.401	-101.748	10.962
5	17.5	46.14	-6.14	0.74	0.01131	-0.105	-0.260	0.657
6	4.9	0.91	206.17	18.26	-0.96080	87.712	12.513	10.735
7	5.3	0.47	1660.77	17.47	-3.64480	280.659	-39.630	17.955
8	4.8	1.76	29.25	17.42	0.17127	-14.443	-12.538	2.562
9	4.7	2.07	-19.06	10.46	0.15617	-7.463	-11.369	1.565
10	6.2	1.06	564.45	54.45	-2.39287	127.725	101.517	17.052
11	4.9	0.99	-244.66	11.17	0.63374	-29.361	-22.886	3.713

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.55, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.37
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.1	0.4	650	19	0.824	1.27

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.11	0.49	649	20	0.854	1.27	0.05	0.30
gr	6.14	0.43	650	19	0.824	1.26	-0.29	0.04
alm	6.24	0.46	654	20	0.851	1.24	-0.72	0.18
phl	6.13	0.43	650	19	0.823	1.26	-0.16	0.02
ann	6.15	0.43	650	19	0.821	1.25	0.56	0.04
east	6.12	0.43	650	19	0.825	1.26	-0.19	0.00
naph	6.17	0.40	649	17	0.819	1.18	-1.49	0.04
mst	6.09	0.44	649	19	0.811	1.26	0.42	0.16
fst	6.26	0.44	664	24	0.814	1.22	0.66	0.51
crd	6.12	0.46	650	19	0.830	1.27	-0.03	0.06
fcrd	6.13	0.43	650	19	0.816	1.27	0.08	0.08
an	6.13	0.43	650	19	0.824	1.27	0.06	0.00
ab	6.14	0.42	650	18	0.823	1.24	0.55	0.01
sp	5.97	0.42	644	18	0.839	1.18	1.43	0.12
herc	6.13	0.37	645	16	0.810	1.09	1.82	0.10

ru	6.[illegible]	[illegible]
ilm	6.[illegible]	[illegible]
cor	6.[illegible]	[illegible]
sill	6.[illegible]	[illegible]
H2O	6.[illegible]	[illegible]

T = 650°C, sd [illegible]
P = 6.1 kbars, [illegible]

**********[illegible]

Sample AJM-WL2 [illegible]

Activities and [illegible]

a	[illegible]	[illegible]
sd(a)/a	0.[illegible]	[illegible]

a	0.[illegible]	[illegible]
sd(a)/a	0.[illegible]	[illegible]

a	[illegible]	
sd(a)/a	0.[illegible]	

Independent se[illegible]
1) 6mst + 75a[illegible] –
2) 2mst + 45a[illegible] –
3) 6fst + 75a[illegible] –
4) 2fst + 45a[illegible] –
5) py + 3herc [illegible] – [illegible]
6) 20py + 9fs [illegible] –
7) 4py + 4gr [illegible] – [illegible]
8) 13gr + 8al[illegible] –
9) 3phl + 3an [illegible] =
10) 7py + 19g[illegible] –
11) 2py + 3an [illegible] –

Calculations f[illegible]
(for x(CO2) = [illegible]

	P(T)	[illegible]
1	5.2	[illegible]
2	5.2	[illegible]
3	5.3	[illegible]
4	5.5	[illegible]
5	17.5	[illegible]
6	4.7	[illegible]
7	4.9	[illegible]
8	5.5	[illegible]
9	4.7	[illegible]
10	6.2	[illegible]
11	4.9	[illegible]

Average PT (f[illegible]

Independent set of reactions

1) 6mst + 75an = 8py + 25gr + 96sill + 12H2O
2) 2mst + 45an = 15gr + 4crd + 40sill + 4H2O
3) 6fst + 75an = 25gr + 8alm + 96sill + 12H2O
4) 2fst + 45an = 15gr + 4fcrd + 40sill + 4H2O
5) py + 3herc = alm + 3sp
6) 20py + 9fst + 40cor = 9mst + 12crd + 36herc
7) 4py + 4gr + 3fst + 16cor = 3mst + 12an + 12herc
8) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
9) 3phl + 3an + 3herc = py + gr + alm + 3east
10) 7py + 19gr + 15phl + 6fst + 12ab = 8alm + 15east + 12naph + 57an
11) 2py + 3ann + 12an + 12ilm = 4gr + 7alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	1.26	156.13	18.93	1.66793	-109.290	-149.191	18.834
2	5.1	1.56	-174.63	10.13	1.13458	-51.406	-83.026	10.935
3	4.8	1.19	241.92	16.93	1.65041	-111.551	-156.773	18.179
4	5.3	1.57	36.56	9.76	1.06259	-51.105	-101.748	10.964
5	17.5	46.14	-6.14	0.74	0.01131	-0.105	-0.260	0.657
6	4.5	0.91	206.17	18.26	-0.96141	87.712	12.513	10.735
7	4.9	0.97	220.34	6.36	-0.59618	30.500	21.149	3.984
8	5.7	0.74	671.03	8.57	-2.13847	94.851	91.789	9.627
9	4.7	2.07	-19.06	10.46	0.15617	-7.463	-11.369	1.565
10	6.2	1.06	564.45	54.45	-2.39287	127.725	101.517	17.052
11	4.9	0.99	-244.66	11.17	0.63374	-29.361	-22.886	3.713

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.55, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.37
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.4	0.5	585	20	0.796	1.60

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.35	0.56	583	22	0.829	1.59	0.33	0.30
gr	5.42	0.49	585	20	0.795	1.60	-0.36	0.04
alm	5.52	0.53	589	22	0.827	1.58	-0.74	0.18
phl	5.43	0.49	585	20	0.794	1.59	-0.46	0.02
ann	5.45	0.48	585	20	0.791	1.55	1.15	0.04
east	5.40	0.49	585	20	0.796	1.60	-0.21	0.00
naph	5.45	0.47	585	19	0.790	1.52	-1.55	0.04
mst	5.33	0.50	584	20	0.783	1.57	0.87	0.14
fst	5.53	0.51	597	26	0.791	1.55	0.71	0.42
crd	5.39	0.52	584	21	0.802	1.60	-0.09	0.06
fcrd	5.45	0.49	585	20	0.786	1.57	1.01	0.09

Independent set of reactions

1) 6mst + 75an = 8py + 25gr + 96sill + 12H2O
2) 2mst + 45an = 15gr + 4crd + 40sill + 4H2O
3) 6fst + 75an = 25gr + 8alm + 96sill + 12H2O
4) 2fst + 45an = 15gr + 4fcrd + 40sill + 4H2O
5) py + 3herc = alm + 3sp
6) 20py + 9fst + 40cor = 9mst + 12crd + 36herc
7) 4py + 4gr + 3fst + 16cor = 3mst + 12an + 12herc
8) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
9) 3phl + 3an + 3herc = py + gr + alm + 3east
10) 7py + 19gr + 15phl + 6fst + 12ab = 8alm + 15east + 12naph + 57an
11) 2py + 3ann + 12an + 12ilm = 4gr + 7alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.8	1.26	156.13	18.93	1.66793	-109.290	-149.191	18.834
2	5.1	1.56	-174.63	10.13	1.13458	-51.406	-83.026	10.935
3	4.8	1.19	241.92	16.93	1.65041	-111.551	-156.773	18.179
4	5.3	1.57	36.56	9.76	1.06259	-51.105	-101.748	10.964
5	17.5	46.14	-6.14	0.74	0.01131	-0.105	-0.260	0.657
6	4.5	0.91	206.17	18.26	-0.96141	87.712	12.513	10.735
7	4.9	0.97	220.34	6.36	-0.59618	30.500	21.149	3.984
8	5.7	0.74	671.03	8.57	-2.13847	94.851	91.789	9.627
9	4.7	2.07	-19.06	10.46	0.15617	-7.463	-11.369	1.565
10	6.2	1.06	564.45	54.45	-2.39287	127.725	101.517	17.052
11	4.9	0.99	-244.66	11.17	0.63374	-29.361	-22.886	3.713

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.55, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.37
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.4	0.5	585	20	0.796	1.60

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.35	0.56	583	22	0.829	1.59	0.33	0.30
gr	5.42	0.49	585	20	0.795	1.60	-0.36	0.04
alm	5.52	0.53	589	22	0.827	1.58	-0.74	0.18
phl	5.43	0.49	585	20	0.794	1.59	-0.46	0.02
ann	5.45	0.48	585	20	0.791	1.55	1.15	0.04
east	5.40	0.49	585	20	0.796	1.60	-0.21	0.00
naph	5.45	0.47	585	19	0.790	1.52	-1.55	0.04
mst	5.33	0.50	584	20	0.783	1.57	0.87	0.14
fst	5.53	0.51	597	26	0.791	1.55	0.71	0.42
crd	5.39	0.52	584	21	0.802	1.60	-0.09	0.06
fcrd	5.45	0.49	585	20	0.786	1.57	1.01	0.09

an	5.41	0.49	585	20	0.796	1.60	0.08	0.00
ab	5.42	0.48	585	20	0.794	1.57	0.57	0.01
sp	5.26	0.48	580	20	0.811	1.51	1.65	0.11
herc	5.43	0.44	581	19	0.781	1.43	2.03	0.08
ru	5.41	0.49	585	20	0.796	1.60	0	0
ilm	5.35	0.41	586	17	0.791	1.34	-2.62	0.03
cor	5.41	0.49	585	20	0.796	1.60	0	0
sill	5.41	0.49	585	20	0.796	1.60	0	0
H2O	5.43	0.49	589	23	0.762	1.58	-0.37	0.15

T = 585°C, sd = 20,
P = 5.4 kbars, sd = 0.5, cor = 0.796, sigfit = 1.60

****

Sample AJM-WL2A

Na-phlogopite, hercynite, spinel, and ilmenite deleted

Activities and their uncertainties

	py	gr	alm	phl	ann	east
a	0.0294	0.00145	0.249	0.106	0.0177	0.0623
sd(a)/a	0.43031	0.70780	0.15000	0.27240	0.49188	0.33787

	mst	fst	crd	fcrd	an
a	0.00482	0.294	0.621	0.0450	0.870
sd(a)/a	0.65106	0.20000	0.05000	0.37242	0.05000

	cor	sill	H2O
a	1.00	1.00	1.00
sd(a)/a	0	0	

Independent set of reactions
1) 2mst + 5crd = 6py + 22sill + 4H2O
2) 2fst + 5fcrd = 6alm + 22sill + 4H2O
3) 6mst + 75an = 8py + 25gr + 96sill + 12H2O
4) 55gr + 6fst + 48fcrd = 40alm + 165an + 12H2O
5) 6gr + 3fst + 6crd + 4cor = 4alm + 3mst + 18an
6) 3phl + 4cor = py + 3east
7) 2py + ann + 6an = 2gr + alm + east + 2crd

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.8	1.19	311.55	3.93	-0.10663	-18.069	-8.110	2.902
2	6.0	0.77	111.90	2.67	-0.02979	-20.141	9.605	2.107
3	5.6	1.25	84.62	18.93	1.85099	-110.367	-149.191	18.822
4	5.3	5.92	699.35	38.64	-4.31965	54.427	437.113	44.051
5	3.8	46.95	270.32	7.06	-0.42278	0.764	21.676	4.845
6	8.6	32.45	25.30	10.43	0.00931	0.444	-5.134	1.371
7	2.5	17.64	-121.09	3.89	0.16462	-0.771	-6.271	1.795

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.3	0.4	659	17	0.789	0.34

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.20	0.45	657	19	0.833	0.32	0.24	0.40
gr	6.28	0.38	659	17	0.787	0.32	-0.31	0.05
alm	6.31	0.43	662	21	0.843	0.33	-0.17	0.32
phl	6.27	0.38	659	17	0.783	0.34	-0.10	0.03
ann	6.29	0.38	659	17	0.774	0.26	0.48	0.09
east	6.25	0.37	658	17	0.789	0.32	-0.21	0.00
mst	6.24	0.40	659	17	0.762	0.34	0.15	0.24
fst	6.27	0.41	660	23	0.807	0.34	0.03	0.41
crd	6.26	0.39	659	17	0.788	0.34	-0.01	0.05
fcrd	6.25	0.38	659	17	0.763	0.34	-0.05	0.18
an	6.26	0.38	659	17	0.789	0.34	0.07	0.00
cor	6.26	0.37	659	17	0.789	0.34	0	0
sill	6.26	0.37	659	17	0.789	0.34	0	0
H2O	6.26	0.37	659	17	0.789	0.34	0	0

T = 659°C, sd = 17,
P = 6.3 kbars, sd = 0.4, cor = 0.789, sigfit = 0.34

****

Sample AJM-WL2A

Na-phlogopite, hercynite, spinel, and ilmenite, and water deleted

Activities and their uncertainties

	py	gr	alm	phl	ann	east
a	0.0294	0.00145	0.249	0.106	0.0177	0.0623
sd(a)/a	0.43031	0.70780	0.15000	0.27240	0.49188	0.33787

	mst	fst	crd	fcrd	an
a	0.00482	0.294	0.621	0.0450	0.870
sd(a)/a	0.65106	0.20000	0.05000	0.37242	0.05000

	cor	sill
a	1.00	1.00
sd(a)/a	0	0

Independent set of reactions
1) 4py + 3fst = 4alm + 3mst
2) 4py + 3fst + 18sill = 3mst + 6fcrd + 10cor
3) 4alm + 3mst + 18sill = 3fst + 6crd + 10cor
4) 3phl + 4cor = py + 3east

5) 4gr + 3phl + 12sill = py + 3east + 12an
6) 2py + ann + 6an = 2gr + alm + east + 2crd

Calculations for the independent set of reactions
(for a(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.8	18.28	42.89	5.64	-0.00876	-1.130	-3.791	2.738
2	4.8	0.88	258.24	6.12	-0.37545	29.414	-16.833	3.483
3	5.9	0.56	-101.45	6.03	-0.25872	30.092	15.041	2.151
4	8.6	32.45	25.30	10.43	0.00931	0.444	-5.134	1.371
5	5.3	1.22	137.88	10.73	-0.44502	21.015	19.343	3.203
6	2.5	17.64	-121.09	3.89	0.16462	-0.771	-6.271	1.795

Average PT (for a(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.46, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.4	0.6	684	59	0.845	0.30

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.38	0.68	681	65	0.868	0.30	0.10	0.48
gr	6.42	0.55	682	61	0.836	0.29	-0.18	0.12
alm	6.43	0.55	684	60	0.809	0.30	-0.04	0.11
phl	6.43	0.55	684	61	0.835	0.30	-0.02	0.06
ann	6.40	0.56	676	63	0.833	0.25	0.33	0.20
east	6.42	0.55	683	59	0.845	0.28	-0.20	0.00
mst	6.46	0.67	687	68	0.883	0.30	-0.07	0.34
fst	6.43	0.57	685	61	0.854	0.30	0.02	0.03
crd	6.43	0.58	685	60	0.844	0.30	0.03	0.05
fcrd	6.48	0.57	698	71	0.834	0.25	-0.31	0.49
an	6.42	0.55	684	59	0.844	0.30	0.04	0.01
cor	6.43	0.55	684	59	0.845	0.30	0	0
sill	6.43	0.55	684	59	0.845	0.30	0	0

T = 684°C, sd = 59,
P = 6.4 kbars, sd = 0.6, cor = 0.845, sigfit = 0.30

****

Sample AJM-WL2B

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 23.13 on Mon 26 Apr,1999

(thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	an	ab	phl	ann
a	0.0372	0.00237	0.192	0.885	0.140	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.22196	0.26867	0.48677

	east	naph	mst	fst	sp	herc	ilm
a	0.0537	0.0144	0.0110	0.209	0.306	0.627	0.967
sd(a)/a	0.35418	0.69648	0.54891	0.20000	0.14464	0.05000	0.05000

	ru	sill	cor	H2O
a	1.00	1.00	1.00	1.00
sd(a)/a	0	0	0	

Independent set of reactions
1) 75an + 6mst = 8py + 25gr + 96sill + 12H2O
2) 75an + 6fst = 25gr + 8alm + 96sill + 12H2O
3) 4py + 3fst + 20cor = 3mst + 12herc + 12sill
4) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
5) 4py + 20gr + 3fst + 48sill = 60an + 3mst + 12herc
6) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
7) 3an + 3phl + 3herc = py + gr + alm + 3east
8) 19gr + 12ab + 15phl + 6mst = py + 57an + 15east + 12naph
9) 4gr + 7alm + 3east + 12ru = 2py + 12an + 3ann + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.1	1.19	84.62	18.93	1.85099	-110.367	-141.220	17.909
2	6.3	1.13	170.41	16.93	1.83347	-112.627	-145.776	17.401
3	2.7	1.88	107.76	5.90	-0.14185	9.930	-1.269	2.447
4	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
5	5.6	0.91	670.68	13.73	-2.41351	112.782	112.295	14.063
6	5.6	0.72	647.19	8.57	-2.07745	94.493	89.078	9.242
7	4.7	2.07	-19.06	10.46	0.15617	-7.463	-11.360	1.570
8	7.1	1.06	478.67	55.09	-2.37535	129.985	93.666	17.479
9	4.6	0.98	244.66	11.17	-0.63374	29.361	24.089	3.634

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.50, point to influential data.

For 95% confidence, fit (= sd(fit)) < 1.42
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.0	0.9	666	29	0.909	1.33

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.07	0.95	667	31	0.917	1.33	-0.10	0.10
gr	5.90	0.97	662	30	0.917	1.31	0.58	0.18
alm	6.86	1.08	692	34	0.946	1.21	-1.15	0.45
an	6.03	0.92	666	30	0.911	1.33	-0.13	0.01
ab	5.99	0.89	664	29	0.910	1.30	0.51	0.01
phl	6.02	0.91	665	29	0.910	1.32	-0.37	0.01
ann	5.89	0.87	661	28	0.913	1.25	1.17	0.04
east	6.03	0.91	666	29	0.910	1.32	-0.36	0.00
naph	5.84	0.84	659	27	0.913	1.20	-1.60	0.05
mst	5.99	0.87	667	28	0.905	1.26	1.10	0.05
fst	6.10	0.92	672	34	0.854	1.32	0.28	0.50
sp	6.11	0.89	667	29	0.906	1.29	0.84	0.04
herc	6.37	0.84	670	26	0.896	1.17	1.48	0.19
ilm	5.81	0.91	661	28	0.909	1.26	-1.05	0.13
ru	6.05	0.91	666	29	0.909	1.33	0	0
sill	6.05	0.91	666	29	0.909	1.33	0	0
cor	6.05	0.91	666	29	0.909	1.33	0	0
H2O	6.05	0.91	666	29	0.909	1.33	0	0

T = 666°C, sd = 29,
P = 6.0 kbars, sd = 0.9, cor = 0.909, sigfit = 1.33

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Sample AJM-WL2B
Na-phlogopite and hercynite deleted
an independent set of reactions has been calculated
Activities and their uncertainties

	py	gr	alm	an	phl	ann
a	0.0372	0.00237	0.192	0.885	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.26867	0.48677

	east	mst	fst	sp	ilm
a	0.0537	0.0110	0.209	0.306	0.967
sd(a)/a	0.35418	0.54891	0.20000	0.14464	0.05000

	ru	sill	cor	H2O
a	1.00	1.00	1.00	1.00
sd(a)/a	0	0	0	

Independent set of reactions
1) 75an + 6mst = 8py + 25gr + 96sill + 12H2O
2) 75an + 6fst = 25gr + 8alm + 96sill + 12H2O
3) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
4) 20gr + 4alm + 3mst + 48sill = 60an + 3fst + 12sp
5) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
6) 3an + 3phl + 3sp = 2py + gr + 3east
7) 5phl + 6ilm + 6sill = 3py + 2ann + 3east + 6ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.1	1.19	84.62	18.93	1.85099	-110.367	-141.220	17.909
2	6.3	1.13	170.41	16.93	1.83347	-112.627	-145.776	17.401
3	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
4	5.8	0.90	560.34	13.89	-2.35074	114.624	114.786	14.082
5	5.6	0.72	647.19	8.57	-2.07745	94.493	89.078	9.242
6	4.8	2.24	-12.92	10.47	0.14485	-7.359	-10.844	1.756
7	10.6	6.30	134.62	10.63	0.01207	-3.166	-15.366	2.326

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.3	0.8	662	23	0.893	0.98

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.34	0.78	664	24	0.900	0.97	-0.31	0.08
gr	6.18	0.83	659	24	0.905	0.97	0.31	0.24
alm	6.70	0.95	676	30	0.934	0.92	-0.56	0.41
an	6.27	0.77	662	23	0.895	0.98	-0.07	0.01
phl	6.23	0.76	660	23	0.894	0.93	-0.55	0.01
ann	6.05	0.77	654	23	0.898	0.69	1.50	0.05
east	6.27	0.76	661	23	0.894	0.96	-0.37	0.00
mst	6.25	0.76	663	23	0.886	0.94	0.61	0.06
fst	6.29	0.77	662	27	0.835	0.98	0.01	0.46
sp	6.41	0.77	664	23	0.889	0.89	0.88	0.08
ilm	6.31	0.91	662	24	0.887	0.98	0.04	0.39
ru	6.28	0.76	662	23	0.893	0.98	0	0
sill	6.28	0.76	662	23	0.893	0.98	0	0
cor	6.28	0.76	662	23	0.893	0.98	0	0
H2O	6.28	0.76	662	23	0.893	0.98	0	0

T = 662°C, sd = 23,
P = 6.3 kbars, sd = 0.8, cor = 0.893, sigfit = 0.98

****

Sample AJM-WL2B
Na-phlogopite and hercynite deleted
an independent set of reactions has been calculated
Activities and their uncertainties

	py	gr	alm	an	phl	ann
a	0.0372	0.00237	0.192	0.885	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.26867	0.48677

	east	mst	fst	sp	ilm
a	0.0537	0.0110	0.209	0.306	0.967
sd(a)/a	0.35418	0.54891	0.20000	0.14464	0.05000

	ru	sill	cor	H2O
a	1.00	1.00	1.00	0.750
sd(a)/a	0	0	0	

Independent set of reactions

1) 75an + 6mst = 8py + 25gr + 96sill + 12H2O
2) 75an + 6fst = 25gr + 8alm + 96sill + 12H2O
3) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
4) 20gr + 4alm + 3mst + 48sill = 60an + 3fst + 12sp
5) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
6) 3an + 3phl + 3sp = 2py + gr + 3east
7) 5phl + 6ilm + 6sill = 3py + 2ann + 3east + 6ru

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.9	1.19	97.39	18.93	1.81415	-110.179	-141.220	17.910
2	6.2	1.13	183.18	16.93	1.79663	-112.439	-145.776	17.401
3	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
4	5.8	0.90	560.34	13.89	-2.35074	114.624	114.786	14.082
5	5.7	0.72	651.45	8.57	-2.08973	94.555	89.078	9.242
6	4.8	2.24	-12.92	10.47	0.14485	-7.359	-10.844	1.756
7	10.6	6.30	134.62	10.63	0.01207	-3.166	-15.366	2.326

Average PT (for x(CO2) = 0.25 and x(H2O) = 0.75)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.1	0.8	642	23	0.890	1.09

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.20	0.82	644	24	0.897	1.08	-0.29	0.08
gr	6.07	0.88	640	25	0.902	1.08	0.21	0.24
alm	6.56	0.95	655	29	0.932	1.03	-0.57	0.41
an	6.13	0.81	642	23	0.892	1.09	-0.05	0.01
phl	6.09	0.75	640	22	0.891	1.02	-0.66	0.01
ann	5.89	0.75	633	22	0.894	0.74	1.71	0.05
east	6.13	0.78	641	23	0.890	1.07	-0.37	0.00
mst	6.10	0.76	643	22	0.883	1.04	0.69	0.06
fst	6.15	0.81	642	27	0.831	1.09	0.02	0.45
sp	6.28	0.75	644	21	0.886	1.00	0.96	0.08
ilm	6.14	0.96	642	25	0.884	1.09	-0.01	0.39

ru	6.14	0.80	642	23	0.890	1.09	0	0
sill	6.14	0.80	642	23	0.890	1.09	0	0
cor	6.14	0.80	642	23	0.890	1.09	0	0
H2O	6.14	0.80	642	23	0.888	1.09	-0.03	0.01

T = 642°C, sd = 23,
P = 6.1 kbars, sd = 0.8, cor = 0.890, sigfit = 1.09

****

Sample AJM-WL2B

Na-phlogopite and hercynite deleted

an independent set of reactions has been calculated
Activities and their uncertainties

	py	gr	alm	an	phl	ann
a	0.0372	0.00237	0.192	0.885	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.26867	0.48677

	east	mst	fst	sp	ilm
a	0.0537	0.0110	0.209	0.306	0.967
sd(a)/a	0.35418	0.54891	0.20000	0.14464	0.05000

	ru	sill	cor	H2O
a	1.00	1.00	1.00	0.500
sd(a)/a	0	0	0	

Independent set of reactions
1) 75an + 6mst = 8py + 25gr + 96sill + 12H2O
2) 75an + 6fst = 25gr + 8alm + 96sill + 12H2O
3) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
4) 20gr + 4alm + 3mst + 48sill = 60an + 3fst + 12sp
5) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
6) 3an + 3phl + 3sp = 2py + gr + 3east
7) 5phl + 6ilm + 6sill = 3py + 2ann + 3east + 6ru

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.8	1.20	126.06	18.93	1.75562	-109.751	-141.220	17.914
2	6.0	1.14	211.85	16.93	1.73810	-112.011	-145.776	17.406
3	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
4	5.8	0.90	560.34	13.89	-2.35074	114.624	114.786	14.082
5	5.7	0.71	661.01	8.57	-2.10924	94.698	89.078	9.243
6	4.8	2.24	-12.92	10.47	0.14485	-7.359	-10.844	1.756
7	10.6	6.30	134.62	10.63	0.01207	-3.166	-15.366	2.326

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.0	0.9	621	24	0.885	1.21

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.05	0.88	623	25	0.892	1.20	-0.26	0.08
gr	5.97	0.94	620	26	0.897	1.21	0.10	0.24
alm	6.41	1.03	634	30	0.928	1.16	-0.59	0.41
an	5.99	0.87	621	25	0.887	1.21	-0.02	0.01
phl	5.93	0.80	619	23	0.886	1.12	-0.79	0.01
ann	5.73	0.72	612	21	0.889	0.80	1.93	0.04
east	5.98	0.85	620	24	0.885	1.19	-0.37	0.00
mst	5.96	0.82	622	23	0.878	1.15	0.78	0.06
fst	6.00	0.87	621	29	0.827	1.21	0.02	0.43
sp	6.15	0.80	623	22	0.881	1.11	1.04	0.08
ilm	5.95	1.03	620	26	0.880	1.21	-0.07	0.38
ru	6.00	0.86	621	24	0.885	1.21	0	0
sill	6.00	0.86	621	24	0.885	1.21	0	0
cor	6.00	0.86	621	24	0.885	1.21	0	0
H2O	6.00	0.86	622	25	0.871	1.20	-0.10	0.06

T = 621°C, sd = 24,
P = 6.0 kbars, sd = 0.9, cor = 0.885, sigfit = 1.21

****

Sample AJM-WL2B

Na-phlogopite and hercynite deleted

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	an	phl	ann
a	0.0372	0.00237	0.192	0.885	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.26867	0.48677

	east	mst	fst	sp	ilm
a	0.0537	0.0110	0.209	0.306	0.967
sd(a)/a	0.35418	0.54891	0.20000	0.14464	0.05000

	ru	sill	cor	H2O
a	1.00	1.00	1.00	0.250
sd(a)/a	0	0	0	

Independent set of reactions

1) 75an + 6mst = 8py + 25gr + 96sill + 12H2O
2) 75an + 6fst = 25gr + 8alm + 96sill + 12H2O
3) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
4) 20gr + 4alm + 3mst + 48sill = 60an + 3fst + 12sp
5) 13gr + 8alm + 2fst + 32ru = 39an + 32ilm + 4H2O
6) 3an + 3phl + 3sp = 2py + gr + 3east
7) 5phl + 6ilm + 6sill = 3py + 2ann + 3east + 6ru

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.3	1.20	156.13	18.93	1.66793	-109.290	-141.220	17.921
2	5.6	1.14	241.92	16.93	1.65041	-111.551	-145.776	17.413

3	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
4	5.8	0.90	560.34	13.89	-2.35074	114.624	114.786	14.082
5	5.9	0.71	671.03	8.57	-2.13847	94.851	89.078	9.245
6	4.8	2.24	-12.92	10.47	0.14485	-7.359	-10.844	1.756
7	10.6	6.30	134.62	10.63	0.01207	-3.166	-15.366	2.326

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.47, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.49
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.7	1.0	582	27	0.873	1.46

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.77	1.01	583	28	0.881	1.46	-0.21	0.08
gr	5.77	1.08	583	28	0.886	1.46	-0.13	0.24
alm	6.14	1.19	594	33	0.921	1.42	-0.61	0.40
an	5.73	0.99	582	27	0.875	1.46	0.03	0.01
phl	5.65	0.90	579	25	0.874	1.34	-1.03	0.01
ann	5.42	0.68	572	19	0.877	0.95	2.38	0.04
east	5.72	0.97	581	26	0.873	1.45	-0.37	0.00
mst	5.68	0.93	583	25	0.866	1.39	0.95	0.05
fst	5.73	0.99	582	31	0.817	1.46	0.02	0.38
sp	5.90	0.93	584	25	0.869	1.36	1.20	0.07
ilm	5.62	1.17	580	28	0.870	1.46	-0.19	0.36
ru	5.73	0.98	582	27	0.873	1.46	0	0
sill	5.73	0.98	582	27	0.873	1.46	0	0
cor	5.73	0.98	582	27	0.873	1.46	0	0
H2O	5.75	0.97	584	28	0.838	1.45	-0.21	0.15

T = 582°C, sd = 27,
P = 5.7 kbars, sd = 1.0, cor = 0.873, sigfit = 1.46

****

Sample AJM-WL2B
Na-phlogopite, hercynite and water deleted
an independent set of reactions has been calculated
Activities and their uncertainties

	py	gr	alm	an	phl	ann
a	0.0372	0.00237	0.192	0.885	0.109	0.0185
sd(a)/a	0.39952	0.67601	0.16120	0.05000	0.26867	0.48677

	east	mst	fst	sp	ilm
a	0.0537	0.0110	0.209	0.306	0.967
sd(a)/a	0.35418	0.54891	0.20000	0.14464	0.05000

	ru	sill	cor
a	1.00	1.00	1.00
sd(a)/a	0	0	0

Independent set of reactions

1) 4py + 3fst = 4alm + 3mst
2) 4alm + 3mst + 20cor = 3fst + 12sp + 12sill
3) 5phl + 4sp + 4sill = 3py + 5east
4) 20gr + 4alm + 3mst + 48sill = 60an + 3fst + 12sp
5) 5mst + 20ilm + 12sill = 4py + 5fst + 8sp + 20ru
6) 4gr + 7alm + 3east + 12ru = 2py + 12an + 3ann + 12ilm

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	16.6	16.56	42.89	5.64	-0.00876	-1.130	-2.278	2.458
2	5.4	1.66	-2.58	6.12	-0.07908	11.771	1.223	2.550
3	1.9	9.13	28.73	17.41	0.04480	-2.807	-8.697	2.591
4	5.8	0.90	560.34	13.89	-2.35074	114.624	114.786	14.082
5	3.6	5.68	-38.33	9.63	0.12198	-4.976	-7.242	3.664
6	4.6	0.98	244.66	11.17	-0.63374	29.361	24.089	3.634

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.2	1.1	795	92	0.767	0.68

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.28	1.10	799	92	0.769	0.66	-0.37	0.05
gr	6.96	1.10	813	94	0.692	0.49	0.91	0.35
alm	7.51	1.23	802	93	0.731	0.63	-0.41	0.30
an	7.16	1.08	797	92	0.757	0.66	-0.20	0.02
phl	7.26	1.15	804	105	0.801	0.68	0.12	0.15
ann	6.78	1.41	749	138	0.872	0.65	0.29	0.55
east	7.16	1.08	794	92	0.768	0.65	-0.37	0.00
mst	7.16	1.11	792	95	0.782	0.68	0.11	0.07
fst	7.18	1.08	794	93	0.771	0.68	-0.04	0.01
sp	7.18	1.08	785	95	0.745	0.65	0.40	0.14
ilm	7.52	1.30	809	96	0.776	0.65	0.33	0.29
ru	7.19	1.08	795	92	0.767	0.68	0	0
sill	7.19	1.08	795	92	0.767	0.68	0	0
cor	7.19	1.08	795	92	0.767	0.68	0	0

T = 795°C, sd = 92,
P = 7.2 kbars, sd = 1.1, cor = 0.767, sigfit = 0.68

****

Sample MP-WL8A

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.44 on Thu 25 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	gr	phl	ann	east	an
a	0.266	0.0261	0.000840	0.118	0.0170	0.0680	0.610
sd(a)/a	0.15000	0.44535	0.73818	0.25859	0.49667	0.32788	0.05000

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.940	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 2phl + ann + 4sill = alm + 3east + 4q
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.5	1.67	28.87	10.50	-0.25084	10.787	16.499	2.009
2	6.1	1.25	137.88	10.73	-0.44502	21.015	17.097	3.293
3	1.9	29.00	-27.00	10.48	0.04240	-0.474	-1.040	1.226
4	5.3	2.24	25.77	10.48	-0.06152	6.924	-0.747	1.577

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.3	1.0	645	88	0.738	0.42

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	6.50	1.14	645	88	0.671	0.33	-0.28	0.28
py	6.16	1.26	628	119	0.835	0.40	0.13	0.32
gr	6.21	1.05	658	93	0.613	0.27	0.41	0.48

Sample AJM-WL3

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 12.15 on Tue 23 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997).

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00439	0.000400	0.381	0.0339	0.0525	0.0365	0.000859
sd(a)/a	0.62940	0.77226	0.15000	0.39930	0.35224	0.39274	11.64144

	an	ab	ilm	sill	q	ru	H2O
a	0.366	0.679	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0.12076	0.05000	0	0	0	0	

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) 2py + 4gr + 3ann + 12sill = 3alm + 3east + 12an
5) py + 2alm + 3east + 6ru = 3phl + 6ilm + 6sill

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.1	1.43	137.88	10.73	-0.44502	21.015	14.006	3.855
2	7.6	1.93	28.87	10.50	-0.25084	10.787	14.823	2.476
3	9.7	7.59	24.61	1.48	0.16677	-11.273	-8.366	11.783
4	8.0	1.54	-23.27	11.14	-0.37449	20.152	26.087	3.992
5	7.3	4.50	-27.19	10.45	-0.05909	3.742	7.145	1.819

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.0	1.0	655	97	0.802	0.60

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.67	1.32	612	139	0.898	0.55	0.28	0.48
gr	7.07	0.97	684	103	0.761	0.39	0.73	0.30
alm	7.50	1.20	659	97	0.686	0.47	-0.48	0.73
phl	6.98	1.03	647	105	0.829	0.59	-0.15	0.11
ann	6.89	1.14	637	118	0.862	0.58	0.16	0.19

east	7.04	0.98	654	98	0.809	0.60	-0.03	0.03
naph	7.04	0.97	654	97	0.803	0.59	-0.26	0.00
an	7.06	0.96	667	100	0.784	0.52	-0.34	0.07
ab	7.05	0.96	655	97	0.802	0.60	0.00	0.00
ilm	7.05	0.96	655	97	0.802	0.60	0	0
sill	7.05	0.96	655	97	0.802	0.60	0	0
q	7.05	0.96	655	97	0.802	0.60	0	0
ru	7.05	0.96	655	97	0.802	0.60	0	0
H2O	7.05	0.96	655	97	0.802	0.60	0	0

T = 655°C, sd = 97,
P = 7.0 kbars, sd = 1.0, cor = 0.802, sigfit = 0.60

****

Sample AJM-WL3

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00439	0.000400	0.381	0.0339	0.0525	0.0365	0.000859
sd(a)/a	0.62940	0.77226	0.15000	0.39930	0.35224	0.39274	11.64144

	an	ab	ilm	sill	q	ru	H2O
a	0.366	0.679	1.00	1.00	1.00	1.00	0.250
sd(a)/a	0.12076	0.05000	0	0	0	0	

Independent set of reactions
1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) naph + 6an = py + 2gr + ab + 3sill + H2O
4) 2py + 4gr + 3ann + 12sill = 3alm + 3east + 12an
5) py + 2alm + 3east + 6ru = 3phl + 6ilm + 6sill

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.1	1.43	137.88	10.73	-0.44502	21.015	14.006	3.855
2	7.6	1.93	28.87	10.50	-0.25084	10.787	14.823	2.476
3	9.1	7.65	30.57	1.48	0.15152	-11.183	-8.366	11.783
4	8.0	1.54	-23.27	11.14	-0.37449	20.152	26.087	3.992
5	7.3	4.50	-27.19	10.45	-0.05909	3.742	7.145	1.819

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.0	1.0	654	96	0.802	0.59

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.66	1.31	611	139	0.898	0.54	0.28	0.48
gr	7.07	0.96	683	103	0.761	0.38	0.73	0.30
alm	7.50	1.20	659	97	0.686	0.46	-0.48	0.73
phl	6.97	1.03	646	105	0.828	0.58	-0.15	0.11
ann	6.88	1.14	636	118	0.861	0.57	0.16	0.19
east	7.04	0.98	654	98	0.809	0.59	-0.03	0.03
naph	7.04	0.96	654	97	0.803	0.58	-0.17	0.00
an	7.06	0.96	667	99	0.784	0.51	-0.34	0.07
ab	7.04	0.96	654	96	0.802	0.59	0.00	0.00
ilm	7.04	0.96	654	96	0.802	0.59	0	0
sill	7.04	0.96	654	96	0.802	0.59	0	0
q	7.04	0.96	654	96	0.802	0.59	0	0
ru	7.04	0.96	654	96	0.802	0.59	0	0
H2O	7.04	0.96	654	96	0.802	0.59	0.00	0.00

T = 654°C, sd = 96,
P = 7.0 kbars, sd = 1.0, cor = 0.802, sigfit = 0.59

****

Sample AJM-WL3

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00439	0.000400	0.381	0.0339	0.0525	0.0365	0.000859
sd(a)/a	0.62940	0.77226	0.15000	0.39930	0.35224	0.39274	11.64144

	an	ab	ilm	sill	q	ru
a	0.366	0.679	1.00	1.00	1.00	1.00
sd(a)/a	0.12076	0.05000	0	0	0	0

Independent set of reactions
1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) 2py + 4gr + 3ann + 12sill = 3alm + 3east + 12an
4) py + 2alm + 3east + 6ru = 3phl + 6ilm + 6sill

Calculations for the independent set of reactions

P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	7.1	1.43	137.88	10.73	-0.44502	21.015	14.006	3.855
2	7.6	1.93	28.87	10.50	-0.25084	10.787	14.823	2.476
3	8.0	1.54	-23.27	11.14	-0.37449	20.152	26.087	3.992
4	7.3	4.50	-27.19	10.45	-0.05909	3.742	7.145	1.819

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.

e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.0	1.0	653	96	0.802	0.71

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.65	1.31	610	139	0.898	0.64	0.29	0.48
gr	7.06	0.96	682	103	0.761	0.45	0.72	0.30
alm	7.49	1.20	658	97	0.686	0.55	-0.48	0.73
phl	6.96	1.03	645	105	0.829	0.70	-0.16	0.11
ann	6.87	1.14	634	118	0.862	0.69	0.17	0.19
east	7.03	0.98	652	98	0.809	0.71	-0.03	0.03
an	7.05	0.96	665	99	0.784	0.62	-0.34	0.07
ilm	7.04	0.96	653	96	0.802	0.71	0	0
sill	7.04	0.96	653	96	0.802	0.71	0	0
q	7.04	0.96	653	96	0.802	0.71	0	0
ru	7.04	0.96	653	96	0.802	0.71	0	0

T = 653°C, sd = 96,
P = 7.0 kbars, sd = 1.0, cor = 0.802, sigfit = 0.71
==========

Sample AJM-LB1

THERMOCALC v2.5, (c) Roger Powell and Tim Holland running at 13.35 on Tue 23 Mar,1999. (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a	0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

	H2O
a	1.00
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	10.0	2.14	288.58	11.28	0.20752	-22.758	-33.298	6.520
4	15.1	78.32	132.61	1.75	-0.01439	-6.645	-2.604	71.706
5	9.0	1.39	51.29	2.53	0.02536	-6.561	-2.046	1.211
6	7.1	1.23	-83.51	10.76	0.56321	-28.498	-28.328	4.594

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	9.0	1.0	787	61	0.762	0.33

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	9.02	1.18	793	76	0.829	0.32	-0.10	0.38
gr	8.96	1.05	787	61	0.744	0.33	-0.05	0.11
alm	8.79	1.42	784	63	0.714	0.32	0.12	0.77
phl	8.89	1.05	783	63	0.775	0.30	-0.23	0.06
ann	8.87	1.06	777	71	0.766	0.30	-0.24	0.36
east	9.06	1.05	796	63	0.776	0.23	0.39	0.07
naph	8.95	1.02	787	61	0.762	0.33	-0.06	0.00
an	8.96	1.04	787	61	0.750	0.33	0.03	0.05
ab	8.95	1.02	787	61	0.762	0.33	0.00	0.00
san	8.95	1.03	787	62	0.767	0.33	0.02	0.02
q	8.95	1.02	787	61	0.762	0.33	0	0
sill	8.95	1.02	787	61	0.762	0.33	0	0
ru	8.95	1.02	787	61	0.762	0.33	0	0
ilm	8.95	1.02	787	61	0.762	0.33	0	0
H2O	8.95	1.02	787	61	0.762	0.33	0	0

T = 787°C, sd = 61,
P = 9.0 kbars, sd = 1.0, cor = 0.762, sigfit = 0.33

****

Sample AJM-LB1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph	
a		0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a		0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

	H2O
a	0.750
sd(a)/a	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	9.8	2.14	292.84	11.28	0.19524	-22.695	-33.298	6.520
4	14.7	78.69	134.74	1.75	-0.02053	-6.614	-2.604	71.706
5	8.5	1.40	53.42	2.53	0.01922	-6.529	-2.046	1.212
6	7.1	1.23	-83.51	10.76	0.56321	-28.498	-28.328	4.594

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.6	0.9	751	54	0.722	0.30

P	sd(P)	T	sd(T)	cor	fit	e*	hat		
py		8.61	1.05	748	66	0.793	0.29	0.06	0.36
gr		8.67	0.95	751	54	0.700	0.29	-0.14	0.11
alm		8.53	1.32	749	56	0.686	0.29	0.09	0.77
phl		8.58	0.94	746	56	0.735	0.24	-0.30.	0.05
ann		8.63	0.95	749	63	0.722	0.29	-0.04	0.36
east		8.72	0.95	757	56	0.737	0.22	0.34	0.06
naph		8.64	0.92	751	54	0.722	0.29	-0.06	0.00
an		8.66	0.94	751	54	0.707	0.29	0.09	0.05
ab		8.64	0.92	751	54	0.722	0.30	0.00	0.00
san		8.64	0.93	751	55	0.726	0.30	-0.00	0.02
q		8.64	0.92	751	54	0.722	0.30	0	0
sill		8.64	0.92	751	54	0.722	0.30	0	0
ru		8.64	0.92	751	54	0.722	0.30	0	0
ilm		8.64	0.92	751	54	0.722	0.30	0	0
H2O		8.64	0.92	751	54	0.722	0.30	-0.00	0.00

T = 751°C, sd = 54,
P = 8.6 kbars, sd = 0.9, cor = 0.722, sigfit = 0.30

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Sample AJM-LB1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a	0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

	H2O
a	0.500
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	9.5	2.16	302.39	11.28	0.17573	-22.553	-33.298	6.521
4	14.3	79.55	139.51	1.75	-0.03029	-6.543	-2.604	71.706
5	8.0	1.42	58.20	2.53	0.00946	-6.458	-2.046	1.213
6	7.1	1.23	-83.51	10.76	0.56321	-28.498	-28.328	4.594

Average PT (for x(CO2) = 0.5 and x(H2O) = 0.5)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.3	0.9	714	48	0.691	0.34

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.22	0.95	704	58	0.764	0.32	0.23	0.35
gr	8.39	0.87	713	48	0.668	0.32	-0.24	0.11
alm	8.27	1.24	712	50	0.668	0.34	0.06	0.77
phl	8.27	0.87	708	49	0.705	0.26	-0.38	0.05
ann	8.38	0.87	719	56	0.687	0.33	0.16	0.37

east	8.40	0.87	718	49	0.706	0.30	0.28	0.06
naph	8.34	0.85	714	48	0.691	0.34	-0.06	0.00
an	8.38	0.87	713	48	0.675	0.33	0.16	0.05
ab	8.34	0.85	714	48	0.691	0.34	0.00	0.00
san	8.35	0.86	714	49	0.695	0.34	-0.02	0.02
q	8.34	0.85	714	48	0.691	0.34	0	0
sill	8.34	0.85	714	48	0.691	0.34	0	0
ru	8.34	0.85	714	48	0.691	0.34	0	0
ilm	8.34	0.85	714	48	0.691	0.34	0	0
H2O	8.34	0.85	714	48	0.693	0.34	-0.01	0.01

T = 714°C, sd = 48,
P = 8.3 kbars, sd = 0.9, cor = 0.691, sigfit = 0.34

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Sample AJM-LB1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a	0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

	H2O
a	0.250
sd(a)/a	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) 2ann + 3an + 3q = gr + 2alm + 2san + 2H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	8.9	2.17	312.42	11.28	0.14650	-22.399	-33.298	6.524
4	13.3	80.49	144.53	1.75	-0.04490	-6.466	-2.604	71.706
5	6.9	1.44	63.21	2.53	-0.00515	-6.381	-2.046	1.216
6	7.1	1.23	-83.51	10.76	0.56321	-28.498	-28.328	4.594

Average PT (for x(CO2) = 0.75 and x(H2O) = 0.25)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.9	0.8	651	40	0.650	0.57

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	7.62	0.83	632	48	0.723	0.47	0.56	0.33
gr	7.93	0.78	650	40	0.624	0.53	-0.45	0.11
alm	7.83	1.13	650	42	0.642	0.57	0.02	0.77
phl	7.76	0.77	644	41	0.665	0.48	-0.53	0.05
ann	7.94	0.77	667	47	0.640	0.48	0.54	0.36
east	7.88	0.77	653	41	0.664	0.56	0.18	0.05
naph	7.85	0.76	651	40	0.650	0.57	-0.05	0.00
an	7.91	0.77	650	40	0.632	0.54	0.30	0.05
ab	7.85	0.76	651	40	0.650	0.57	0.00	0.00
san	7.86	0.76	652	41	0.653	0.57	-0.06	0.02
q	7.85	0.76	651	40	0.650	0.57	0	0
sill	7.85	0.76	651	40	0.650	0.57	0	0
ru	7.85	0.76	651	40	0.650	0.57	0	0
ilm	7.85	0.76	651	40	0.650	0.57	0	0
H2O	7.86	0.76	652	41	0.653	0.57	-0.06	0.02

T = 651°C, sd = 40,
P = 7.9 kbars, sd = 0.8, cor = 0.650, sigfit = 0.57

****

Sample AJM-LB1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a	0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

	H2O
a	0.100
sd(a)/a	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 7phl + 12an = 5py + 4gr + 3east + 4san + 4H2O
4) 2naph + 3an + 3q = 2py + gr + 2ab + 2H2O
5) ann + 6an = 2gr + alm + san + 3sill + H2O
6) 3phl + 12an + 12ilm = py + 4gr + 4alm + 3east + 12ru

Calculations for the independent set of reactions
(for x(CO2) = 0.9 and x(H2O) = 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	7.8	2.18	316.65	11.28	0.11356	-22.330	-33.298	6.530
4	11.5	80.93	146.64	1.75	-0.06137	-6.432	-2.604	71.706
5	6.0	1.35	-9.03	1.74	0.16316	-11.124	-9.199	2.049
6	7.1	1.23	-83.51	10.76	0.56321	-28.498	-28.328	4.594

Average PT (for x(CO2) = 0.9 and x(H2O) = 0.1)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	7.2	0.7	570	34	0.606	1.01

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	6.90	0.72	543	40	0.681	0.80	1.05	0.32
gr	7.38	0.68	569	33	0.576	0.93	-0.77	0.11
alm	7.28	1.01	571	35	0.609	1.01	-0.03	0.77
phl	7.14	0.67	562	34	0.623	0.90	-0.77	0.06
ann	7.38	0.67	597	39	0.592	0.78	1.07	0.31
east	7.26	0.68	571	35	0.619	1.01	0.05	0.04
naph	7.25	0.67	570	34	0.606	1.01	-0.05	0.00
an	7.34	0.68	569	33	0.585	0.96	0.52	0.05
ab	7.25	0.67	570	34	0.606	1.01	0.00	0.00
san	7.26	0.67	572	34	0.609	1.01	-0.11	0.02
q	7.25	0.67	570	34	0.606	1.01	0	0
sill	7.25	0.67	570	34	0.606	1.01	0	0
ru	7.25	0.67	570	34	0.606	1.01	0	0
ilm	7.25	0.67	570	34	0.606	1.01	0	0

H2O	7.29	0.67	576	36	0.615	1.00	-0.21	0.07

T = 570°C, sd = 34,
P = 7.2 kbars, sd = 0.7, cor = 0.606, sigfit = 1.01

****

Sample AJM-LB1

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00150	4.00e-5	0.511	0.00855	0.0782	0.0208	0.000279
sd(a)/a	0.70574	0.83949	0.15000	0.49419	0.29487	0.43947	35.84229

	an	ab	san	q	sill	ru	ilm
a	0.210	0.772	0.840	1.00	1.00	1.00	1.00
sd(a)/a	0.18703	0.05000	0.05000	0	0	0	0

a
sd(a)/a

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 2phl + ann + 4sill = alm + 3east + 4q
4) py + 3east + 12q + 12ilm = 4alm + 3phl + 12ru
5) py + 3east + 3ab + 12q + 12ilm = 4alm + 3naph + 3san + 12ru

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	7.7	2.19	28.87	10.50	-0.25084	10.787	14.738	2.918
2	5.8	1.65	137.88	10.73	-0.44502	21.015	17.967	4.555
3	19.9	33.92	-27.00	10.48	0.04240	-0.474	-0.220	1.681
4	5.7	2.75	-25.77	10.48	0.06152	-6.924	1.148	2.190
5	0.63	131.55	13.41	10.77	0.05062	-5.934	-8.866	107.539

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.7	1.4	754	133	0.883	0.34

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.56	2.09	742	202	0.948	0.34	0.05	0.55
gr	8.66	1.42	748	138	0.868	0.33	-0.13	0.18
alm	8.57	1.62	754	133	0.761	0.33	0.09	0.78
phl	8.48	1.51	734	143	0.899	0.27	-0.29	0.11
ann	8.75	1.63	761	155	0.914	0.34	-0.06	0.13
east	8.84	1.47	770	138	0.892	0.24	0.34	0.06
naph	8.67	1.41	754	133	0.883	0.34	-0.06	0.00
an	8.66	1.42	750	136	0.873	0.33	0.09	0.08
ab	8.67	1.41	754	133	0.883	0.34	0.00	0.00
san	8.67	1.41	754	133	0.883	0.34	-0.00	0.00
q	8.67	1.41	754	133	0.883	0.34	0	0
sill	8.67	1.41	754	133	0.883	0.34	0	0
ru	8.67	1.41	754	133	0.883	0.34	0	0
ilm	8.67	1.41	754	133	0.883	0.34	0	0

T = 754°C, sd = 133,
P = 8.7 kbars, sd = 1.4, cor = 0.883, sigfit = 0.34

Sample AJM-LB2

THERMOCALC v2.5, (c) Roger Powell and Tim Holland running at 13.35 on Tue 23 Mar,1999. (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

Activities and their uncertainties

	py	gr	alm	phl	ann	east	naph
a	0.00662	1.00e-5	0.479	0.0375	0.0487	0.0462	0.00220
sd(a)/a	0.59375	1.39248	0.15000	0.39009	0.36281	0.36990	4.54545

	an	ab	sill	ru	ilm	q
a	0.186	0.806	1.00	1.00	1.00	1.00
sd(a)/a	0.19853	0.05000	0	0	0	0

Independent set of reactions

1) 4gr + 3phl + 12sill = py + 3east + 12an
2) py + 2gr + 3east + 6q = 3phl + 6an
3) alm + 3east + 4q = 2phl + ann + 4sill
4) 3phl + 6sill + 6ilm = py + 2alm + 3east + 6ru

Calculations for the independent set of reactions

P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)	
1	4.6	2.23	137.88	10.73	-0.44502	21.015	21.504	6.297
2	5.9	2.54	28.87	10.50	-0.25084	10.787	17.346	3.483
3	17.0	30.92	27.00	10.48	-0.04240	0.474	0.375	1.412
4	9.7	4.39	27.19	10.45	0.05909	-3.742	-5.868	1.745

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.0	1.2	717	115	0.818	0.62

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	8.08	1.67	726	175	0.915	0.62	-0.04	0.50
gr	7.97	1.16	702	118	0.805	0.43	-0.64	0.12
alm	7.69	1.41	723	117	0.583	0.56	0.24	0.86
phl	7.90	1.25	706	126	0.844	0.60	-0.16	0.12
ann	8.16	1.45	735	149	0.886	0.60	-0.12	0.24
east	8.07	1.18	726	118	0.825	0.57	0.27	0.03
an	7.99	1.16	711	116	0.812	0.55	0.28	0.02

sill	7.99	1.16	717	115	0.818	0.62	0	0
ru	7.99	1.16	717	115	0.818	0.62	0	0
ilm	7.99	1.16	717	115	0.818	0.62	0	0
q	7.99	1.16	717	115	0.818	0.62	0	0

T = 717°C, sd = 115,
P = 8.0 kbars, sd = 1.2, cor = 0.818, sigfit = 0.62

****

Sample MP-LB132

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.19 on Thu 25 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	phl	ann	east	mu	cel
a	0.321	0.00134	0.0283	0.0630	0.0370	0.700	0.0140
sd(a)/a	0.15000	0.71249	0.43505	0.33660	0.40013	0.10000	0.46641

	q	sill	ilm	ru	H2O
a	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0	0	0	0	

Independent set of reactions
1) 3east + 6q = py + phl + 2mu
2) 7phl + 12sill = 5py + 3east + 4mu
3) 11phl + 12sill = 5py + 7east + 4cel
4) ann + q + 2sill = alm + mu
5) alm + ann + 6ru = mu + 3q + 6ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.4	4.71	45.25	10.42	-0.02569	-3.172	-1.003	1.476
2	5.1	5.35	170.64	11.07	0.00528	-6.904	-19.438	4.855
3	8.0	7.04	211.24	24.91	0.11289	-7.901	-34.014	6.850
4	4.8	1.54	-17.73	1.24	0.02011	-1.967	1.271	0.382
5	6.7	1.94	-18.21	1.33	-0.02010	1.588	3.545	0.382

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	6.3	0.9	679	112	0.717	0.88

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	6.29	1.29	678	115	0.355	0.88	-0.02	0.93
py	6.74	1.10	743	135	0.797	0.73	-0.73	0.36
phl	6.26	1.00	680	121	0.752	0.88	0.02	0.11

ann	6.22	1.03	673	136	0.772	0.88	0.07	0.35
east	6.27	0.96	680	114	0.726	0.88	0.04	0.03
mu	6.21	0.95	670	114	0.720	0.84	-0.31	0.01
cel	5.98	0.97	646	115	0.733	0.55	1.28	0.08
q	6.26	0.94	679	112	0.717	0.88	0	0
sill	6.26	0.94	679	112	0.717	0.88	0	0
ilm	6.26	0.94	679	112	0.717	0.88	0	0
ru	6.26	0.94	679	112	0.717	0.88	0	0

T = 679°C, sd = 112,
P = 6.3 kbars, sd = 0.9, cor = 0.717, sigfit = 0.88

****

Sample MP-LB132

Celadonite Excluded

Activities and their uncertainties

	alm	py	phl	ann	east	mu
a	0.321	0.00134	0.0283	0.0630	0.0370	0.700
sd(a)/a	0.15000	0.71249	0.43505	0.33660	0.40013	0.10000

	q	sill	ilm	ru	H2O
a	1.00	1.00	1.00	1.00	1.00
sd(a)/a	0	0	0	0	

Independent set of reactions
1) 7phl + 12sill = 5py + 3east + 4mu
2) 3east + 6q = py + phl + 2mu
3) ann + q + 2sill = alm + mu
4) alm + ann + 6ru = mu + 3q + 6ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.1	5.35	170.64	11.07	0.00528	-6.904	-19.438	4.855
2	5.4	4.71	45.25	10.42	-0.02569	-3.172	-1.003	1.476
3	4.8	1.54	-17.73	1.24	0.02011	-1.967	1.271	0.382
4	6.7	1.94	-18.21	1.33	-0.02010	1.588	3.545	0.382

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.40, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.9	0.9	635	106	0.708	0.40

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	5.78	1.26	638	108	0.364	0.38	0.08	0.93
py	6.14	1.09	668	135	0.809	0.28	-0.31	0.42
phl	5.95	0.93	643	113	0.736	0.37	0.15	0.08
ann	5.72	1.00	603	132	0.774	0.27	0.34	0.39
east	5.91	0.91	637	108	0.716	0.39	0.06	0.02
mu	5.89	0.89	632	107	0.708	0.36	-0.15	0.01
q	5.90	0.89	635	106	0.708	0.40	0	0
sill	5.90	0.89	635	106	0.708	0.40	0	0
ilm	5.90	0.89	635	106	0.708	0.40	0	0
ru	5.90	0.89	635	106	0.708	0.40	0	0

T = 635°C, sd = 106,
P = 5.9 kbars, sd = 0.9, cor = 0.708, sigfit = 0.40

****

Sample MP-LB134

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.24 on Thu 25 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

	alm	py	gr	phl	ann	east	an
a	0.525	0.00134	2.00e-5	0.0164	0.0790	0.0210	0.280
sd(a)/a	0.15000	0.71249	1.10521	0.45617	0.29335	0.43870	0.15552

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions

1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) 3alm + 2gr + 3east + 6q = 2py + 3ann + 6an
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.2	2.33	28.87	10.50	-0.25084	10.787	19.875	3.142
2	4.3	1.87	137.88	10.73	-0.44502	21.015	22.130	5.210
3	3.5	2.23	190.02	10.92	-0.32137	11.650	6.679	3.240
4	8.2	2.76	25.77	10.48	-0.06152	6.924	-3.787	2.198

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.5	1.9	737	159	0.809	1.23

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	7.87	1.76	745	137	0.700	1.05	0.61	0.37
py	9.43	2.48	830	232	0.911	1.15	-0.38	0.57

gr	8.62	1.51	691	134	0.769	0.74	-1.34	0.25
phl	8.68	1.94	755	170	0.833	1.21	0.26	0.11
ann	8.70	2.07	757	184	0.853	1.22	-0.15	0.13
east	8.49	1.90	736	165	0.819	1.23	-0.02	0.05
an	8.55	1.62	719	141	0.794	1.07	0.56	0.04
q	8.50	1.86	737	159	0.809	1.23	0	0
sill	8.50	1.86	737	159	0.809	1.23	0	0
ilm	7.61	2.03	715	144	0.759	1.09	-0.53	0.41
ru	8.50	1.86	737	159	0.809	1.23	0	0

T = 737°C, sd = 159,
P = 8.5 kbars, sd = 1.9, cor = 0.809, sigfit = 1.23

****

Sample MP-LB134

Grossular Excluded

Activities and their uncertainties

	alm	py	phl	ann	east
a	0.525	0.00134	0.0164	0.0790	0.0210
sd(a)/a	0.15000	0.71249	0.45617	0.29335	0.43870

	q	sill	ilm	ru
a	1.00	1.00	0.960	1.00
sd(a)/a	0	0	0.05000	0

Independent set of reactions
1) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm
2) 2alm + py + 3east + 6ru = 3phl + 6sill + 6ilm
3) alm + 2py + 3ann + 12ru = 3east + 12q + 12ilm

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	8.2	2.76	25.77	10.48	-0.06152	6.924	-3.787	2.198
2	7.7	4.89	-27.19	10.45	-0.05909	3.742	6.917	2.072
3	9.8	3.21	-135.38	10.90	0.00901	6.061	9.410	2.218

Average PT

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.96

however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.6	1.4	670	119	0.742	0.18

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	8.64	1.64	670	123	0.482	0.18	-0.00	0.50
py	8.70	2.02	677	195	0.885	0.18	-0.03	0.61
phl	8.69	1.49	676	131	0.776	0.14	0.09	0.12
ann	8.62	1.57	668	140	0.801	0.18	0.01	0.14
east	8.59	1.43	666	123	0.754	0.13	-0.11	0.05
q	8.63	1.40	670	119	0.742	0.18	0	0
sill	8.63	1.40	670	119	0.742	0.18	0	0
ilm	8.63	1.85	670	119	0.599	0.18	-0.00	0.50
ru	8.63	1.40	670	119	0.742	0.18	0	0

T = 670°C, sd = 119,
P = 8.6 kbars, sd = 1.4, cor = 0.742, sigfit = 0.18

****

Sample MP-LB135

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 10.31 on Thu 25 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

an independent set of reactions has been calculated

Activities and their uncertainties

alm	py	gr	phl	ann	east	an	
a	0.534	0.00136	3.00e-5	0.0212	0.0760	0.0240	0.280
sd(a)/a	0.15000	0.71162	0.96549	0.43800	0.29903	0.42850	0.15552

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) py + 2gr + 3east + 6q = 3phl + 6an
2) 4gr + 3phl + 12sill = py + 3east + 12an
3) py + ann = alm + phl
4) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.5	2.19	28.87	10.50	-0.25084	10.787	19.419	2.913
2	5.0	1.71	137.88	10.73	-0.44502	21.015	20.154	4.720
3	3.2	22.97	-53.72	1.00	0.02351	-0.288	4.696	0.900
4	8.6	2.71	25.77	10.48	-0.06152	6.924	-4.209	2.146

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.36, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.73
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.2	1.7	703	144	0.805	1.22

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	7.63	1.59	707	122	0.709	1.02	0.64	0.35
py	9.20	2.20	798	202	0.906	1.11	-0.44	0.56
gr	8.37	1.41	658	123	0.755	0.77	-1.23	0.28

phl	8.45	1.76	723	152	0.828	1.18	0.32	0.10
ann	8.45	1.89	723	166	0.849	1.20	-0.17	0.13
east	8.22	1.74	700	148	0.813	1.21	-0.07	0.04
an	8.30	1.47	683	126	0.782	1.04	0.59	0.07
q	8.25	1.71	703	144	0.805	1.22	0	0
sill	8.25	1.71	703	144	0.805	1.22	0	0
ilm	7.39	1.84	680	129	0.766	1.06	-0.56	0.39
ru	8.25	1.71	703	144	0.805	1.22	0	0

T = 703°C, sd = 144,
P = 8.2 kbars, sd = 1.7, cor = 0.805, sigfit = 1.22

****

Sample MP-LB135

Grossular Excluded

Activities and their uncertainties

	alm	py	phl	ann	east
a	0.534	0.00136	0.0212	0.0760	0.0240
sd(a)/a	0.15000	0.71162	0.43800	0.29903	0.42850

	q	sill	ilm	ru	H2O
a	1.00	1.00	0.960	1.00	1.00
sd(a)/a	0	0	0.05000	0	

Independent set of reactions
1) py + ann = alm + phl
2) 4alm + 3phl + 12ru = py + 3east + 12q + 12ilm
3) 2alm + py + 3east + 6ru = 3phl + 6sill + 6ilm

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	3.2	22.97	-53.72	1.00	0.02351	-0.288	4.696	0.900
2	8.6	2.71	25.77	10.48	-0.06152	6.924	-4.209	2.146
3	7.1	4.81	-27.19	10.45	-0.05909	3.742	7.238	2.016

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.33, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.96
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	8.4	1.3	634	110	0.720	0.28

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
alm	8.40	1.54	634	113	0.450	0.28	-0.01	0.50
py	8.48	1.86	644	180	0.873	0.27	-0.04	0.61
phl	8.47	1.38	643	121	0.756	0.21	0.14	0.12
ann	8.37	1.46	631	130	0.784	0.28	0.02	0.14
east	8.34	1.33	629	113	0.732	0.20	-0.16	0.04
q	8.39	1.30	634	110	0.720	0.28	0	0
sill	8.39	1.30	634	110	0.720	0.28	0	0
ilm	8.38	1.74	634	110	0.576	0.28	-0.00	0.50
ru	8.39	1.30	634	110	0.720	0.28	0	0

T = 634°C, sd = 110,
P = 8.4 kbars, sd = 1.3, cor = 0.720, sigfit = 0.28

Sample MP-HP12

THERMOCALC v2.5, © Roger Powell and Tim Holland running at 15.32 on Tue 23 Mar,1999 (thermodynamic dataset produced at 15.57 on Fri 26 Sep,1997)

An independent set of reactions has been calculated

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	1.00
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions

1) 3an + pa = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) 11phl + 12sill = 5py + 7east + 4cel
5) ann + q + 2sill = alm + mu
6) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(H2O) = 1.0)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.7	1.64	28.64	0.66	0.04440	-4.042	-5.492	0.908
2	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
3	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
4	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
5	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
6	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.7	1.3	725	41	0.856	0.52

P	sd(P)	T	sd(T)	cor	fit	e*	hat

py	5.90	1.39	731	44	0.875	0.47	-0.40	0.15
gr	5.34	1.58	716	46	0.886	0.48	0.34	0.41
alm	5.64	1.34	724	42	0.860	0.51	0.11	0.04
phl	5.83	1.32	729	42	0.863	0.46	0.39	0.04
ann	5.57	1.40	722	43	0.864	0.50	-0.21	0.16
east	5.71	1.31	725	42	0.860	0.52	0.05	0.02
an	5.58	1.39	722	43	0.867	0.51	-0.14	0.07
ab	5.69	1.30	724	43	0.840	0.52	0.05	0.07
mu	5.65	1.33	724	42	0.861	0.51	0.09	0.03
pa	5.61	1.33	713	58	0.760	0.50	-0.17	0.87
cel	5.87	1.32	730	42	0.861	0.41	-0.71	0.05
q	5.70	1.29	725	41	0.856	0.52	0	0
sill	5.70	1.29	725	41	0.856	0.52	0	0
H2O	5.70	1.29	725	41	0.856	0.52	0	0

T = 725°C, sd = 41,
P = 5.7 kbars, sd = 1.3, cor = 0.856, sigfit = 0.52

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	0.750
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions
1) 3an + pa = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) 11phl + 12sill = 5py + 7east + 4cel
5) ann + q + 2sill = alm + mu
6) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(CO2) = 0.25 and x(H2O) = 0.75)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.3	1.64	29.71	0.66	0.04133	-4.026	-5.492	0.908
2	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
3	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
4	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
5	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
6	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.5	1.3	693	39	0.857	0.41

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.57	1.34	697	42	0.876	0.40	-0.23	0.15
gr	5.17	1.53	687	44	0.888	0.38	0.28	0.41
alm	5.43	1.30	693	40	0.860	0.41	0.05	0.04
phl	5.55	1.28	696	40	0.864	0.37	0.30	0.04
ann	5.39	1.35	692	40	0.864	0.41	-0.10	0.16
east	5.45	1.27	693	39	0.861	0.41	0.00	0.02
an	5.36	1.35	691	41	0.868	0.40	-0.12	0.07
ab	5.45	1.25	693	41	0.841	0.41	0.03	0.07
mu	5.41	1.29	692	40	0.862	0.41	0.08	0.03
pa	5.40	1.29	686	55	0.761	0.40	-0.12	0.86
cel	5.60	1.28	698	40	0.862	0.30	-0.63	0.05
q	5.45	1.25	693	39	0.857	0.41	0	0
sill	5.45	1.25	693	39	0.857	0.41	0	0
H2O	5.45	1.25	693	39	0.856	0.41	0.01	0.00

T = 693°C, sd = 39,
P = 5.5 kbars, sd = 1.3, cor = 0.857, sigfit = 0.41

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	0.500
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions
1) 3an + pa = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) 11phl + 12sill = 5py + 7east + 4cel
5) ann + q + 2sill = alm + mu
6) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(CO2) = 0.5 and x(H2O) = 0.5)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.9	1.66	32.10	0.66	0.03645	-3.990	-5.492	0.908
2	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
3	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
4	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
5	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
6	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.2	1.2	660	36	0.857	0.32

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	5.21	1.28	660	38	0.875	0.32	-0.03	0.15
gr	4.99	1.46	656	40	0.887	0.30	0.21	0.40
alm	5.20	1.24	660	36	0.860	0.32	-0.01	0.04
phl	5.26	1.23	662	37	0.863	0.30	0.19	0.04
ann	5.20	1.30	660	37	0.864	0.32	0.01	0.16
east	5.18	1.21	660	36	0.860	0.32	-0.05	0.02
an	5.13	1.29	659	37	0.868	0.31	-0.09	0.07
ab	5.19	1.20	660	37	0.840	0.32	0.02	0.07
mu	5.17	1.23	659	36	0.861	0.32	0.06	0.03
pa	5.17	1.23	657	50	0.756	0.32	-0.06	0.84
cel	5.32	1.22	663	36	0.862	0.20	-0.54	0.05
q	5.20	1.20	660	36	0.857	0.32	0	0
sill	5.20	1.20	660	36	0.857	0.32	0	0
H2O	5.19	1.20	660	36	0.849	0.32	0.01	0.03

T = 660°C, sd = 36,
P = 5.2 kbars, sd = 1.2, cor = 0.857, sigfit = 0.32

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an

a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	0.330
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions

1) 3an + pa = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) 11phl + 12sill = 5py + 7east + 4cel
5) ann + q + 2sill = alm + mu
6) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(CO2) = 0.67 and x(H2O) = 0.33)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	5.3	1.67	33.86	0.66	0.03191	-3.963	-5.492	0.909
2	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
3	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
4	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
5	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
6	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	4.9	1.1	626	33	0.856	0.29

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.84	1.23	623	35	0.875	0.27	0.19	0.15
gr	4.81	1.40	623	37	0.887	0.28	0.13	0.41
alm	4.96	1.19	626	34	0.860	0.28	-0.07	0.04
phl	4.95	1.17	626	34	0.864	0.28	0.08	0.04
ann	5.01	1.24	627	34	0.864	0.27	0.14	0.15
east	4.91	1.16	625	33	0.860	0.28	-0.11	0.02
an	4.89	1.23	625	35	0.868	0.28	-0.05	0.07
ab	4.93	1.15	626	34	0.840	0.29	-0.00	0.07
mu	4.91	1.18	625	34	0.861	0.28	0.04	0.03
pa	4.93	1.17	626	45	0.754	0.29	0.01	0.82

cel	5.03	1.17	628	34	0.862	0.20	-0.44	0.05
q	4.93	1.15	626	33	0.856	0.29	0	0
sill	4.93	1.15	626	33	0.856	0.29	0	0
H2O	4.93	1.15	626	34	0.843	0.29	-0.00	0.05

T = 626°C, sd = 33,
P = 4.9 kbars, sd = 1.1, cor = 0.856, sigfit = 0.29

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	0.250
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions
1) 3an + pa = gr + ab + 3sill + H2O
2) 3east + 6q = py + phl + 2mu
3) 7phl + 12sill = 5py + 3east + 4mu
4) 11phl + 12sill = 5py + 7east + 4cel
5) ann + q + 2sill = alm + mu
6) py + gr + mu = phl + 3an

Calculations for the independent set of reactions
(for x(CO2) = 0.75 and x(H2O) = 0.25)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	4.9	1.68	34.60	0.66	0.02915	-3.952	-5.492	0.909
2	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
3	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
4	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
5	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
6	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	4.7	1.1	602	31	0.855	0.32

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.59	1.19	598	34	0.873	0.27	0.35	0.15
gr	4.68	1.36	601	36	0.886	0.32	0.07	0.41
alm	4.80	1.15	603	32	0.859	0.31	-0.12	0.04
phl	4.74	1.14	602	32	0.862	0.32	-0.01	0.04
ann	4.87	1.20	604	33	0.863	0.29	0.24	0.15
east	4.71	1.13	601	32	0.858	0.31	-0.15	0.02
an	4.73	1.20	602	33	0.867	0.32	-0.03	0.07
ab	4.75	1.11	602	33	0.839	0.32	-0.02	0.07
mu	4.74	1.15	602	32	0.860	0.32	0.02	0.03
pa	4.77	1.14	605	43	0.752	0.32	0.06	0.79
cel	4.83	1.14	604	32	0.861	0.27	-0.37	0.05
q	4.75	1.11	602	31	0.855	0.32	0	0
sill	4.75	1.11	602	31	0.855	0.32	0	0
H2O	4.75	1.11	602	33	0.836	0.32	-0.02	0.08

T = 602°C, sd = 31,
P = 4.7 kbars, sd = 1.1, cor = 0.855, sigfit = 0.32

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill	H2O
a	0.730	0.680	0.239	0.00430	1.00	1.00	0.100
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0	

Independent set of reactions
1) 3east + 6q = py + phl + 2mu
2) 7phl + 12sill = 5py + 3east + 4mu
3) 11phl + 12sill = 5py + 7east + 4cel
4) ann + q + 2sill = alm + mu
5) py + gr + mu = phl + 3an
6) py + 2pa + 3cel = 3east + 2ab + 9q + 2H2O

Calculations for the independent set of reactions
(for x(CO2) = 0.9 and x(H2O) = 0.1)

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
2	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
3	4.3	7.09	211.24	24.91	0.11289	-7.901	-38.205	6.912
4	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
5	5.1	1.28	-8.19	0.96	-0.11257	6.980	9.864	1.220

6	6.0	2.38	41.93	10.73	-0.22285	8.144	14.738	2.228

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.43, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.54
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	4.2	1.0	526	27	0.841	0.67

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	3.78	1.08	516	29	0.861	0.47	0.92	0.15
gr	4.26	1.24	528	31	0.874	0.66	-0.14	0.41
alm	4.27	1.05	528	28	0.844	0.63	-0.29	0.04
phl	4.05	1.04	523	28	0.850	0.64	-0.33	0.04
ann	4.42	1.09	531	28	0.847	0.58	0.58	0.14
east	4.10	1.02	525	27	0.844	0.65	-0.28	0.01
an	4.19	1.09	527	28	0.853	0.67	0.06	0.07
ab	4.16	1.01	527	28	0.826	0.67	-0.06	0.05
mu	4.16	1.04	526	28	0.845	0.67	-0.03	0.02
pa	4.22	1.03	535	36	0.745	0.64	0.23	0.66
cel	4.17	1.03	527	28	0.847	0.67	-0.11	0.05
q	4.15	1.01	526	27	0.841	0.67	0	0
sill	4.15	1.01	526	27	0.841	0.67	0	0
H2O	4.18	1.02	529	31	0.793	0.66	-0.13	0.22

T = 526°C, sd = 27,
P = 4.2 kbars, sd = 1.0, cor = 0.841, sigfit = 0.67

****

MP-HP12

Activities and their uncertainties

	py	gr	alm	phl	ann	east	an
a	0.00139	8.00e-5	0.350	0.0245	0.0770	0.0310	0.390
sd(a)/a	0.71033	0.82411	0.15000	0.42687	0.29712	0.40732	0.11163

	ab	mu	pa	cel	q	sill
a	0.730	0.680	0.239	0.00430	1.00	1.00
sd(a)/a	0.05000	0.10000	0.17374	0.55814	0	0

Independent set of reactions

1) 3east + 6q = py + phl + 2mu
2) 7phl + 12sill = 5py + 3east + 4mu
3) phl + east + 6q = py + 2cel
4) ann + q + 2sill = alm + mu
5) gr + alm + mu = ann + 3an

Calculations for the independent set of reactions

	P(T)	sd(P)	a	sd(a)	b	c	ln_K	sd(ln_K)
1	6.1	4.73	45.25	10.42	-0.02569	-3.172	-0.638	1.490
2	5.6	5.31	170.64	11.07	0.00528	-6.904	-18.893	4.816
3	4.7	3.06	65.55	3.95	0.02811	-3.671	-10.294	1.449
4	4.3	1.43	-17.73	1.24	0.02011	-1.967	1.130	0.348
5	4.7	0.97	45.53	1.38	-0.13608	7.267	5.479	0.955

Average PT (for x(H2O) = 1.0)

Single end-member diagnostic information

avP, avT, sd's, cor, fit are result of doubling the uncertainty on ln a :
a ln a is suspect if any are v different from lsq values.
e* are ln a residuals normalised to ln a uncertainties :
large absolute values, say >2.5, point to suspect info.
hat are the diagonal elements of the hat matrix :
large values, say >0.45, point to influential data.
For 95% confidence, fit (= sd(fit)) < 1.61
however a larger value may be OK - look at the diagnostics!

	avP	sd	avT	sd	cor	fit
lsq	5.0	1.4	632	104	0.761	0.33

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
py	4.72	1.89	611	146	0.873	0.30	0.15	0.55
gr	4.88	1.53	633	105	0.662	0.31	0.14	0.45
alm	4.99	1.40	629	107	0.724	0.32	-0.06	0.08
phl	5.07	1.54	639	117	0.806	0.32	0.10	0.15
ann	5.00	1.40	626	112	0.672	0.32	0.12	0.32
east	4.94	1.44	629	107	0.774	0.32	-0.10	0.04
an	4.95	1.44	632	105	0.728	0.32	-0.06	0.07
mu	4.97	1.41	632	105	0.746	0.32	0.04	0.03
cel	5.18	1.47	646	109	0.783	0.21	-0.46	0.13
q	4.98	1.40	632	104	0.761	0.33	0	0
sill	4.98	1.40	632	104	0.761	0.33	0	0

T = 632°C, sd = 104,
P = 5.0 kbars, sd = 1.4, cor = 0.761, sigfit = 0.33

Figure DR1

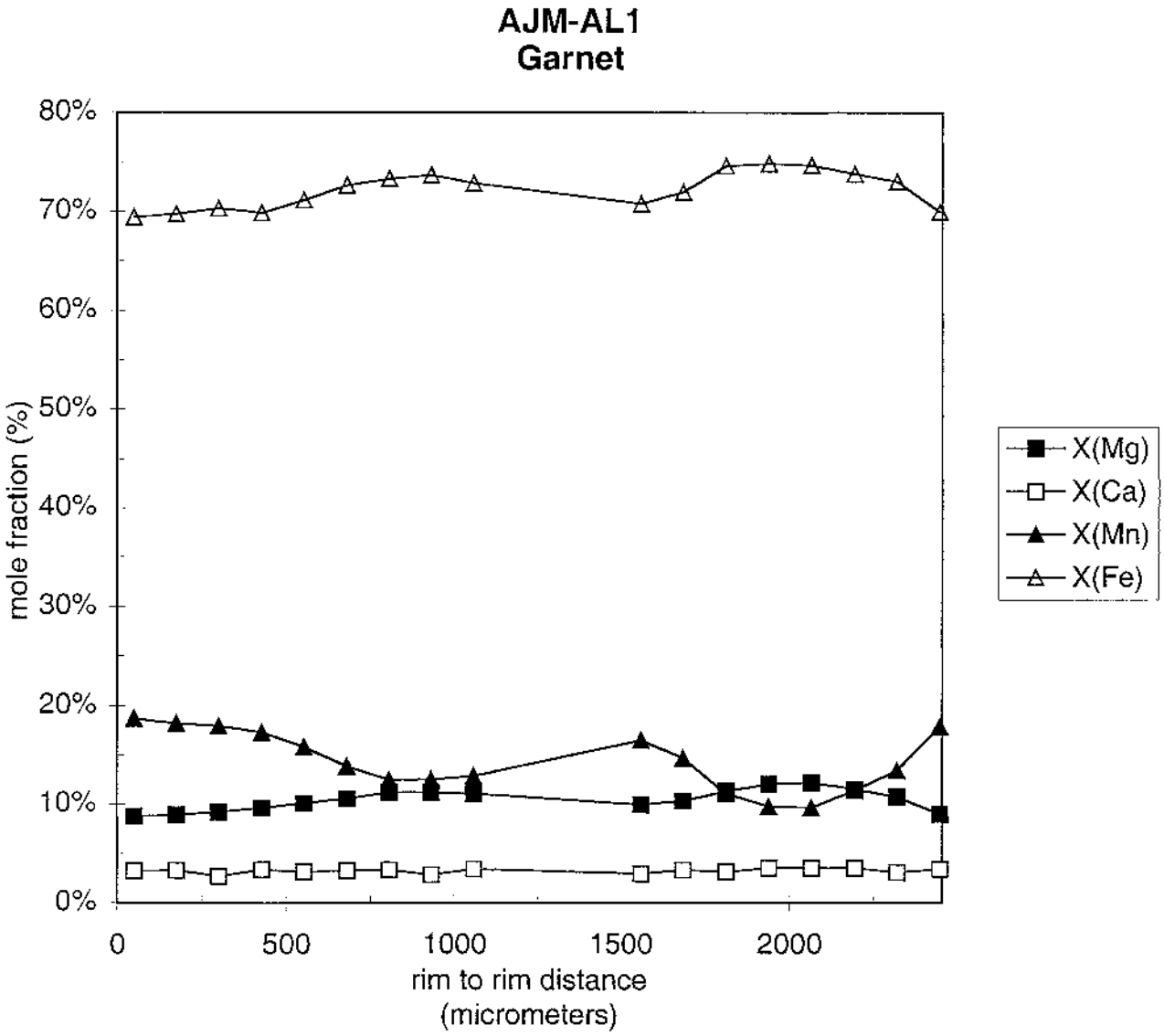
AJM-AL1
Garnet
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
500
1000
1500
2000
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR2

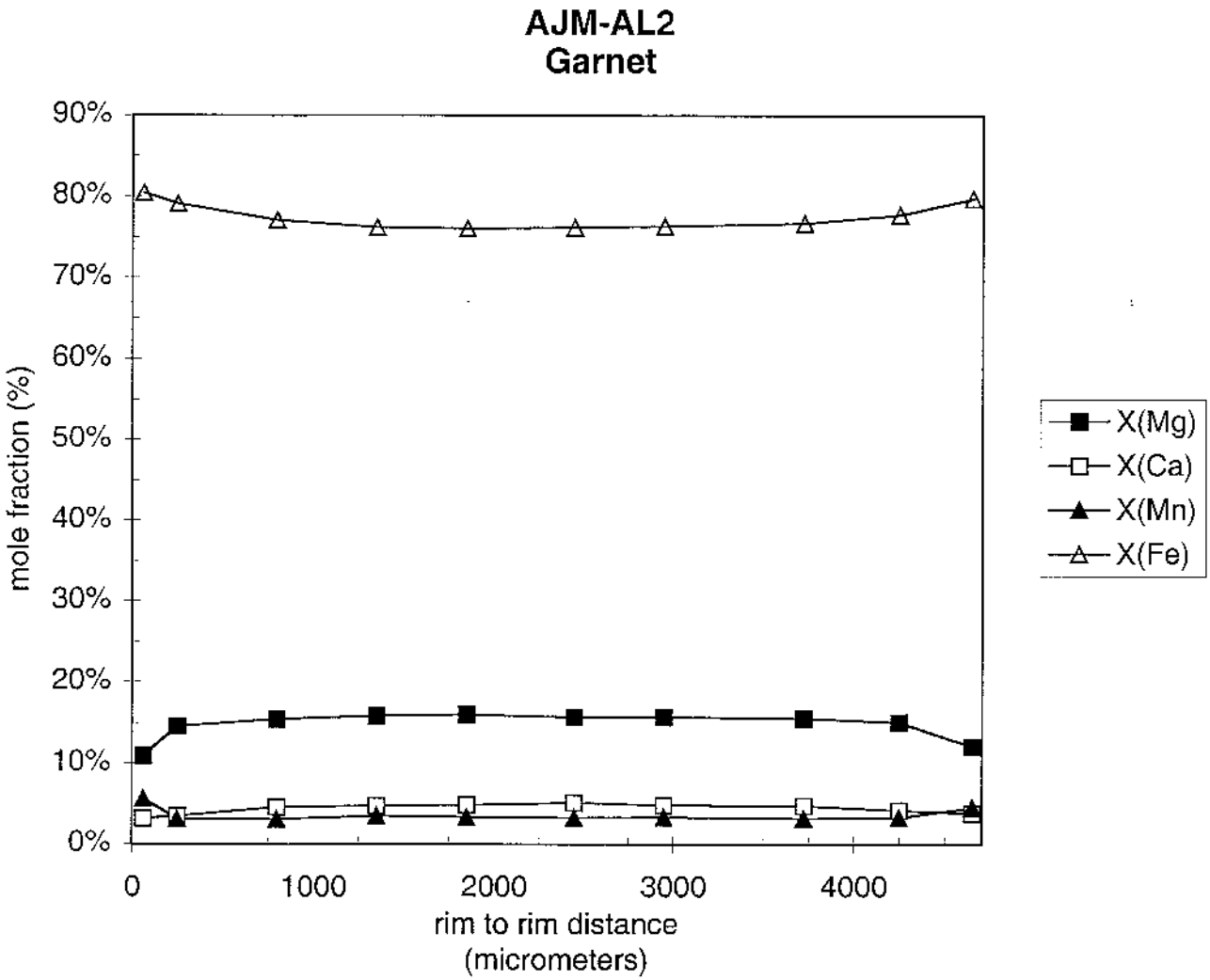
AJM-AL2
Garnet
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
1000
2000
3000
4000
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR3

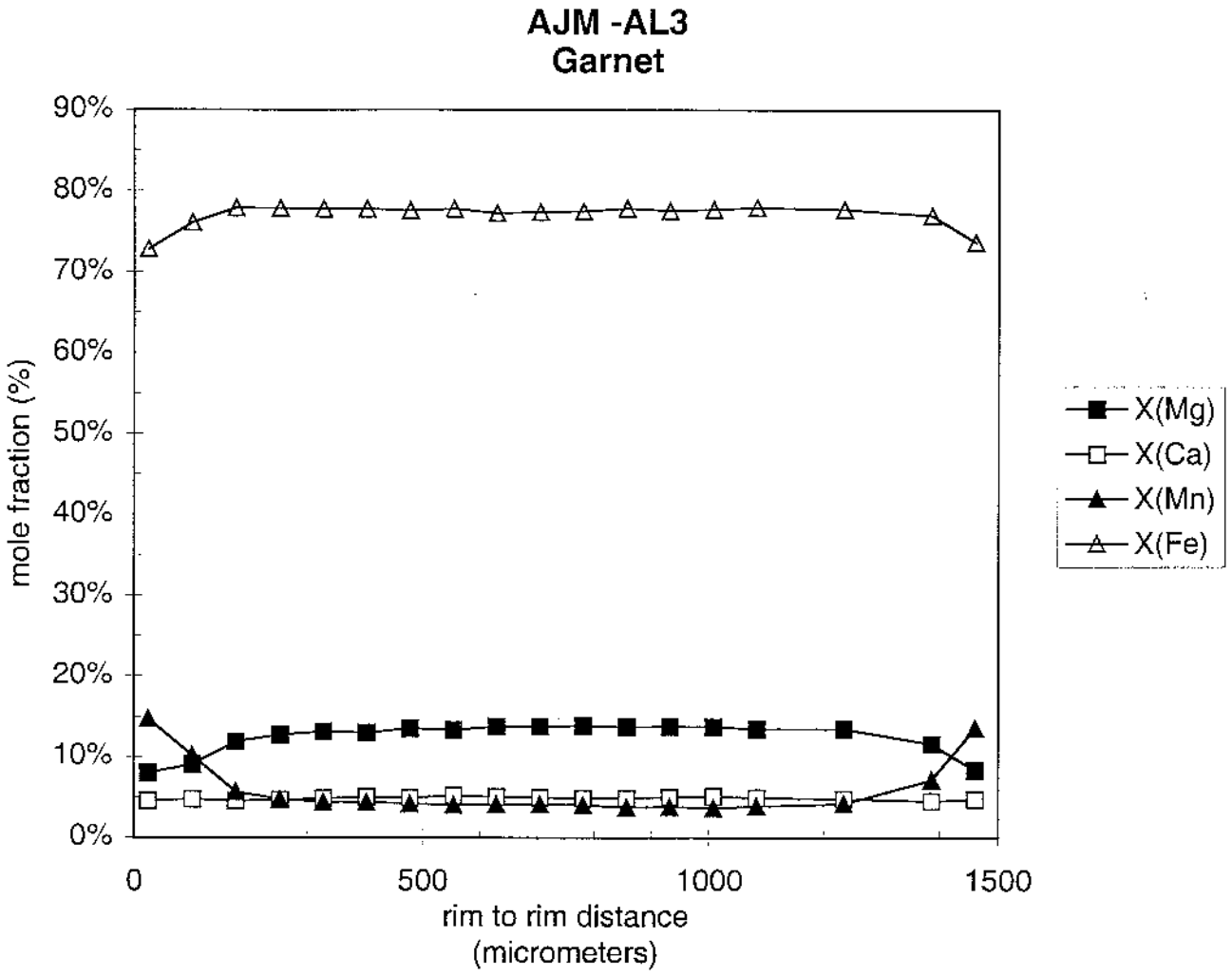

Fig. 3a

Figure DR4

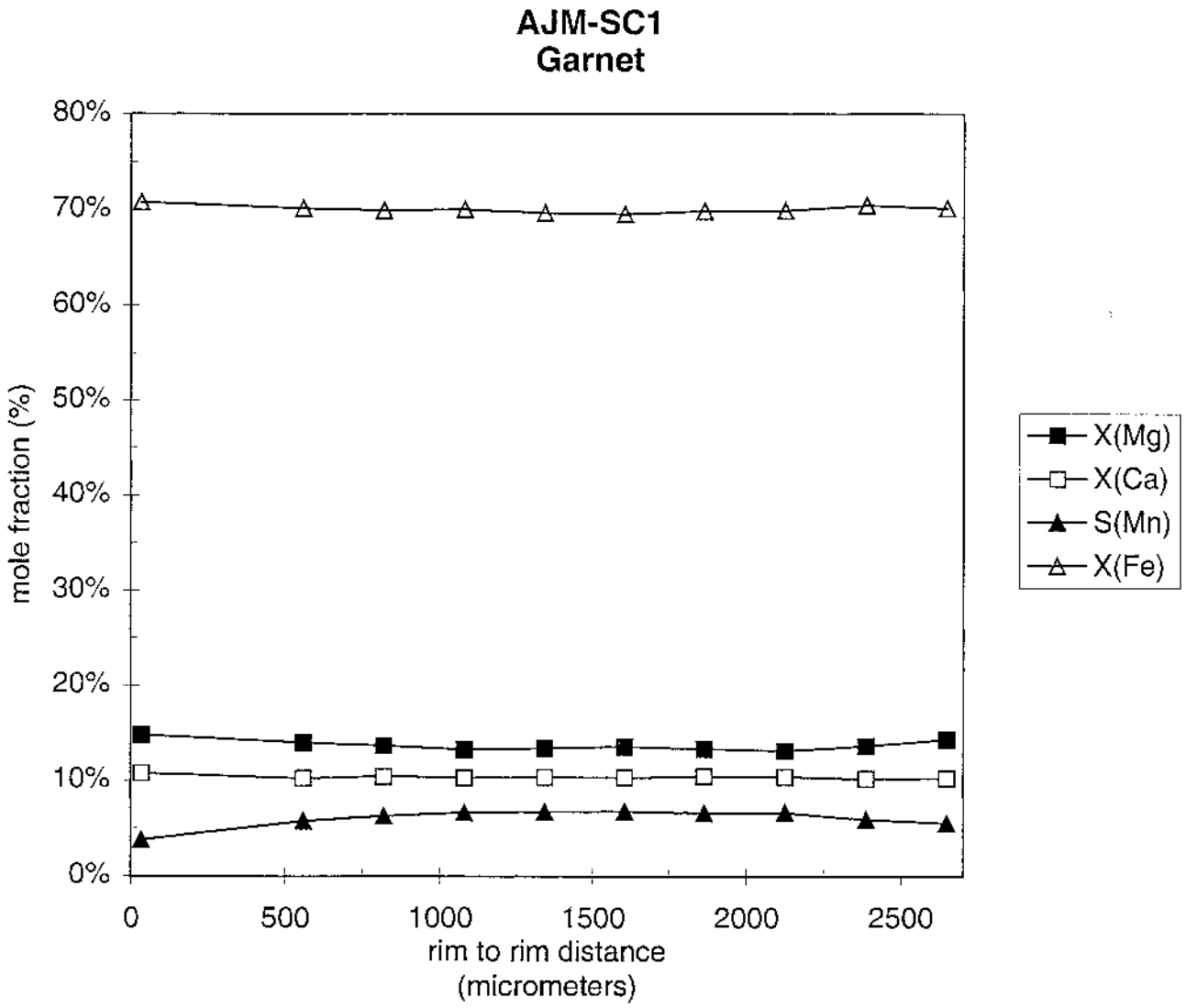

Fig. 3b

Figure DR5

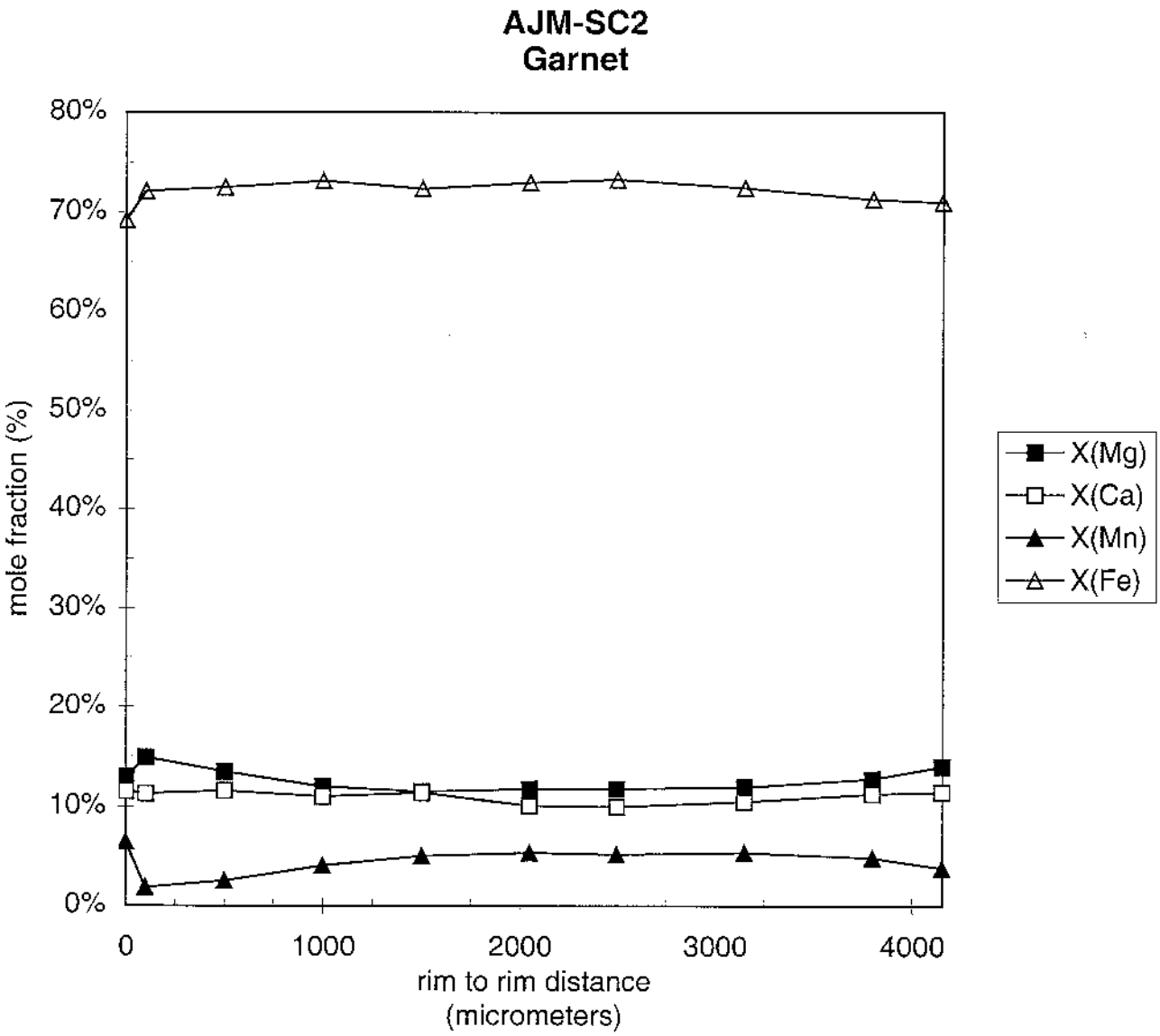
AJM-SC2
Garnet
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
1000
2000
3000
4000
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR6

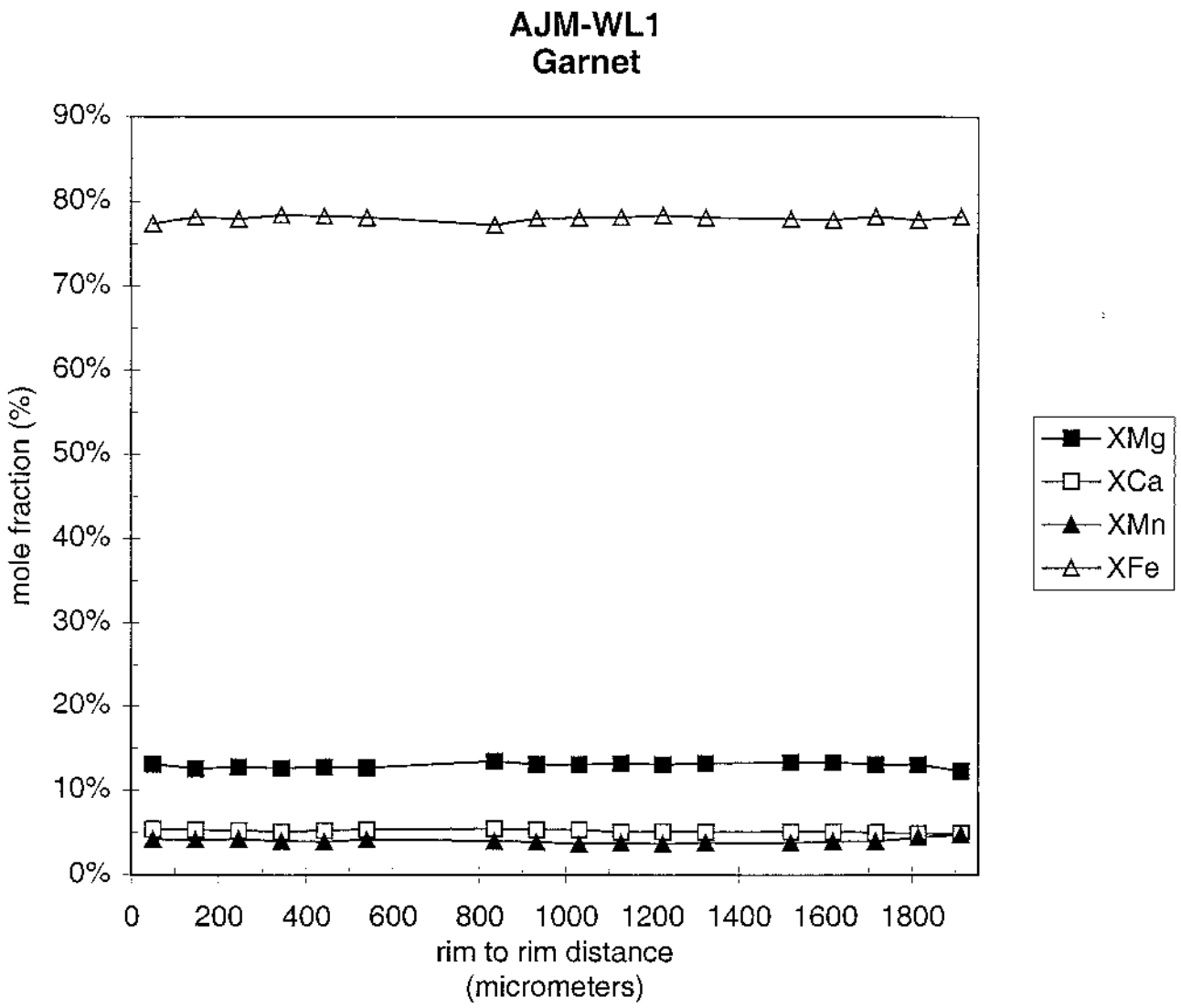
AJM-WL1
Garnet
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
200
400
600
800
1000
1200
1400
1600
1800
rim to rim distance
(micrometers)
XMg
XCa
XMn
XFe

Figure DR7

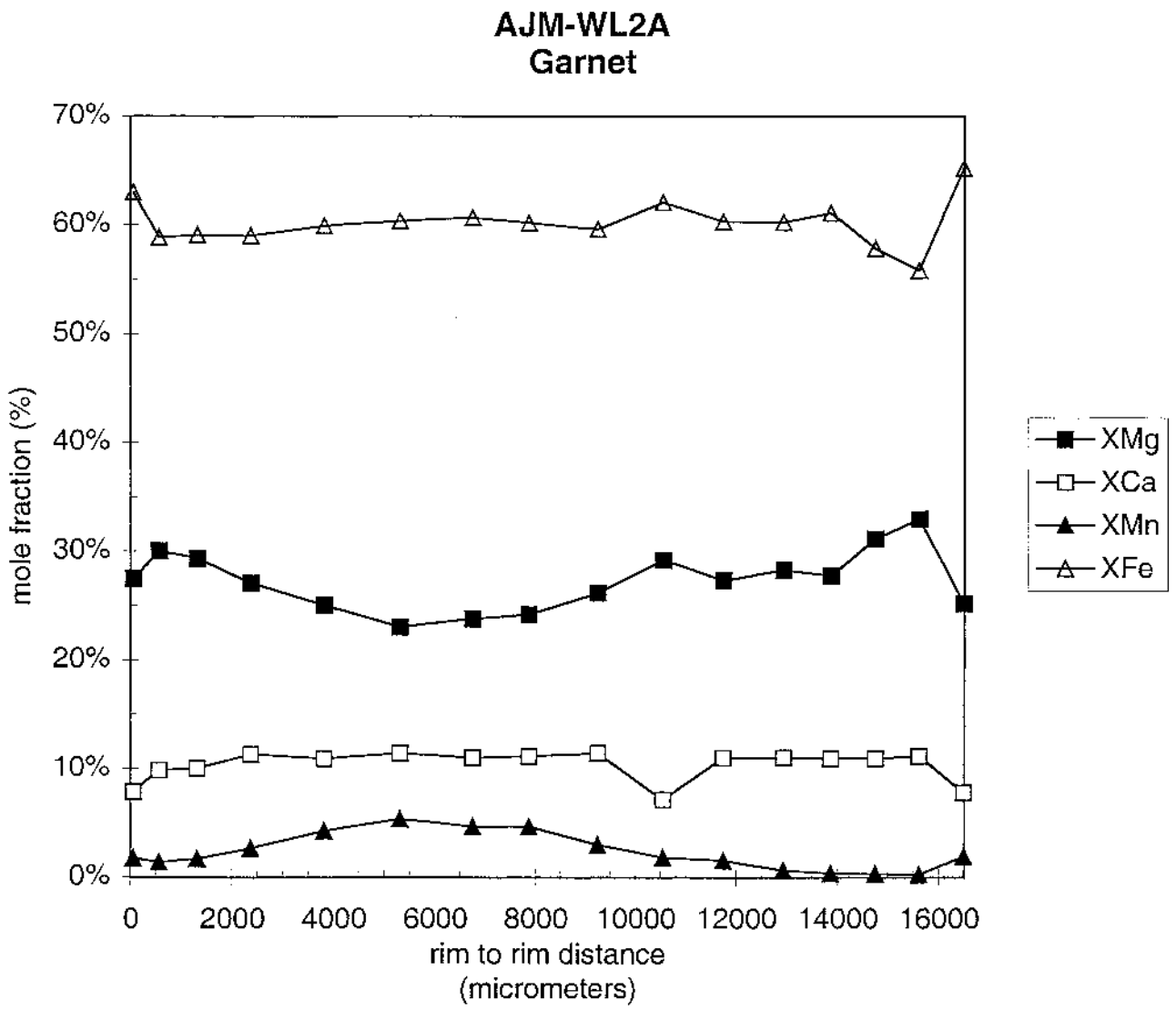
AJM-WL2A
Garnet
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
2000
4000
6000
8000
10000
12000
14000
16000
rim to rim distance
(micrometers)
XMg
XCa
XMn
XFe

Figure DR8

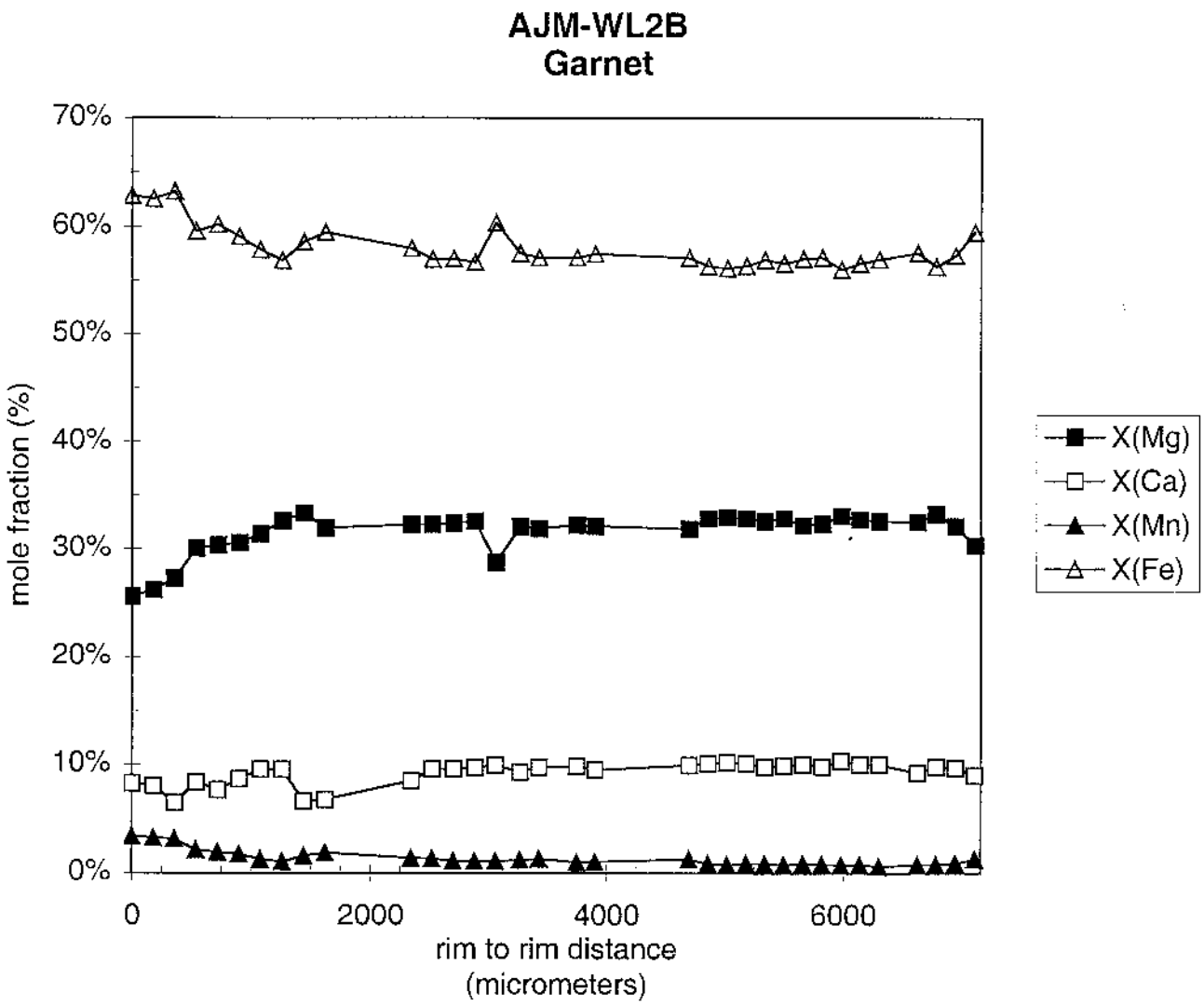
AJM-WL2B
Garnet
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
2000
4000
6000
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR9

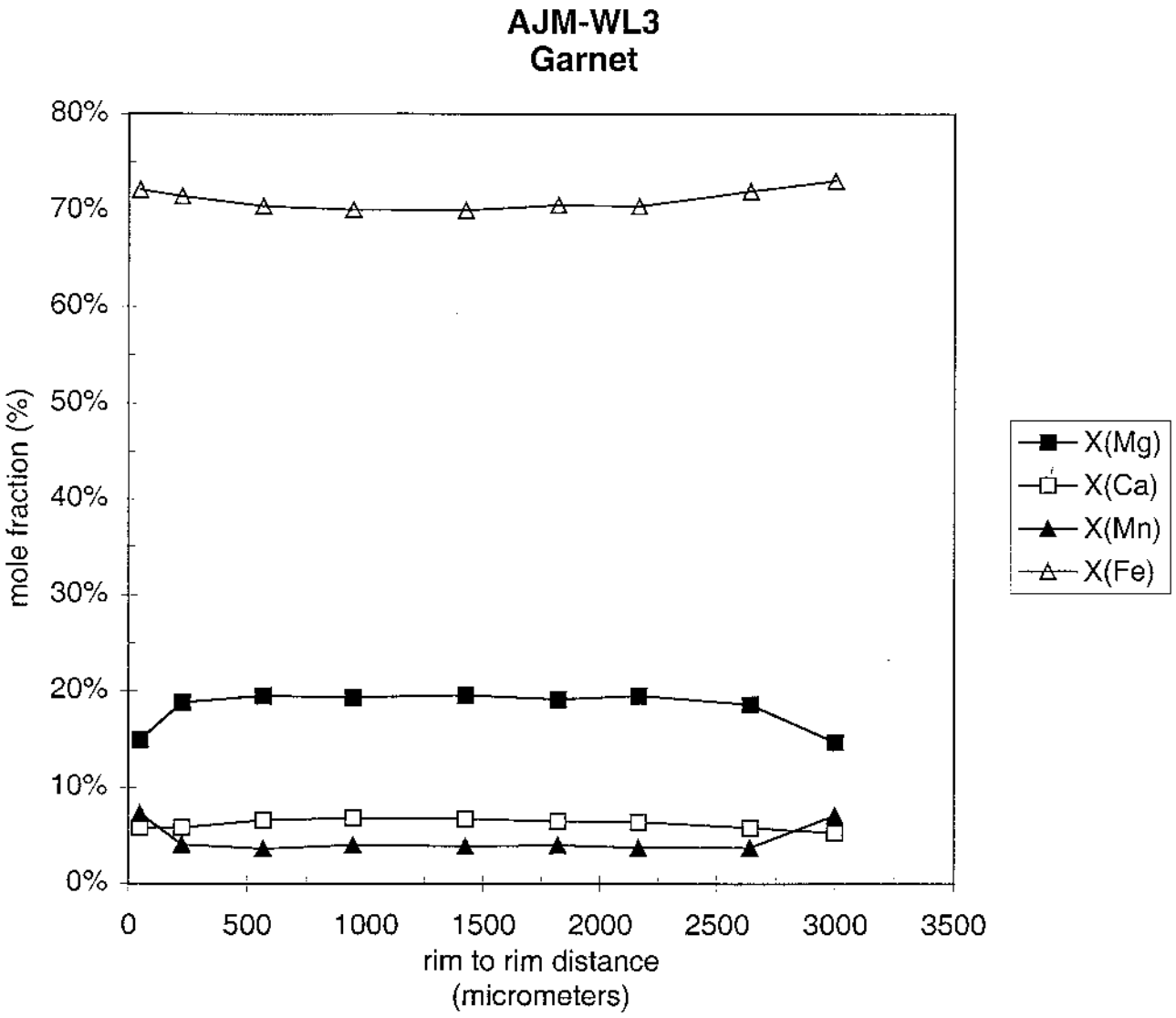
AJM-WL3
Garnet
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
500
1000
1500
2000
2500
3000
3500
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR10

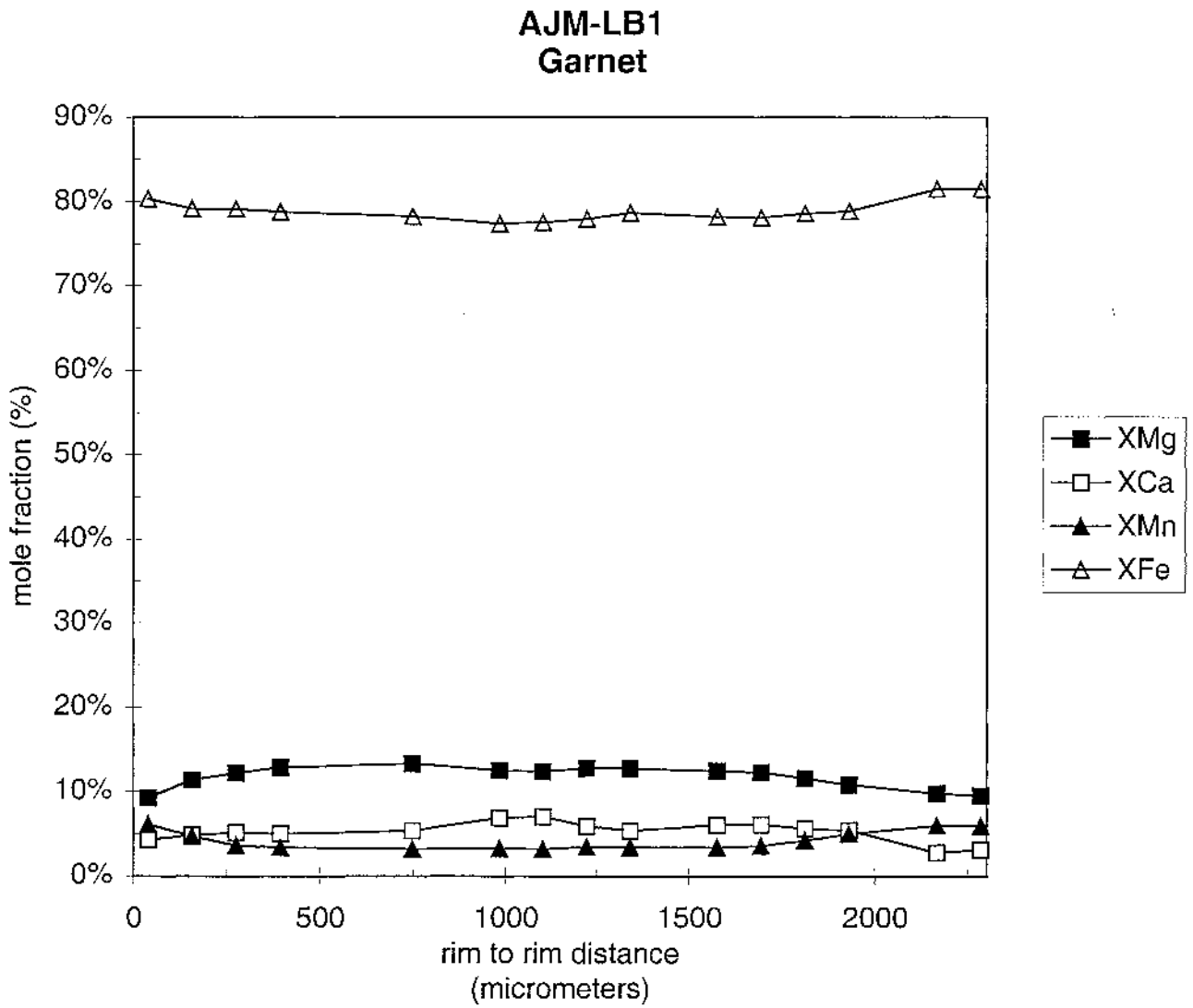
AJM-LB1
Garnet
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
500
1000
1500
2000
rim to rim distance
(micrometers)
XMg
XCa
XMn
XFe

Figure DR11

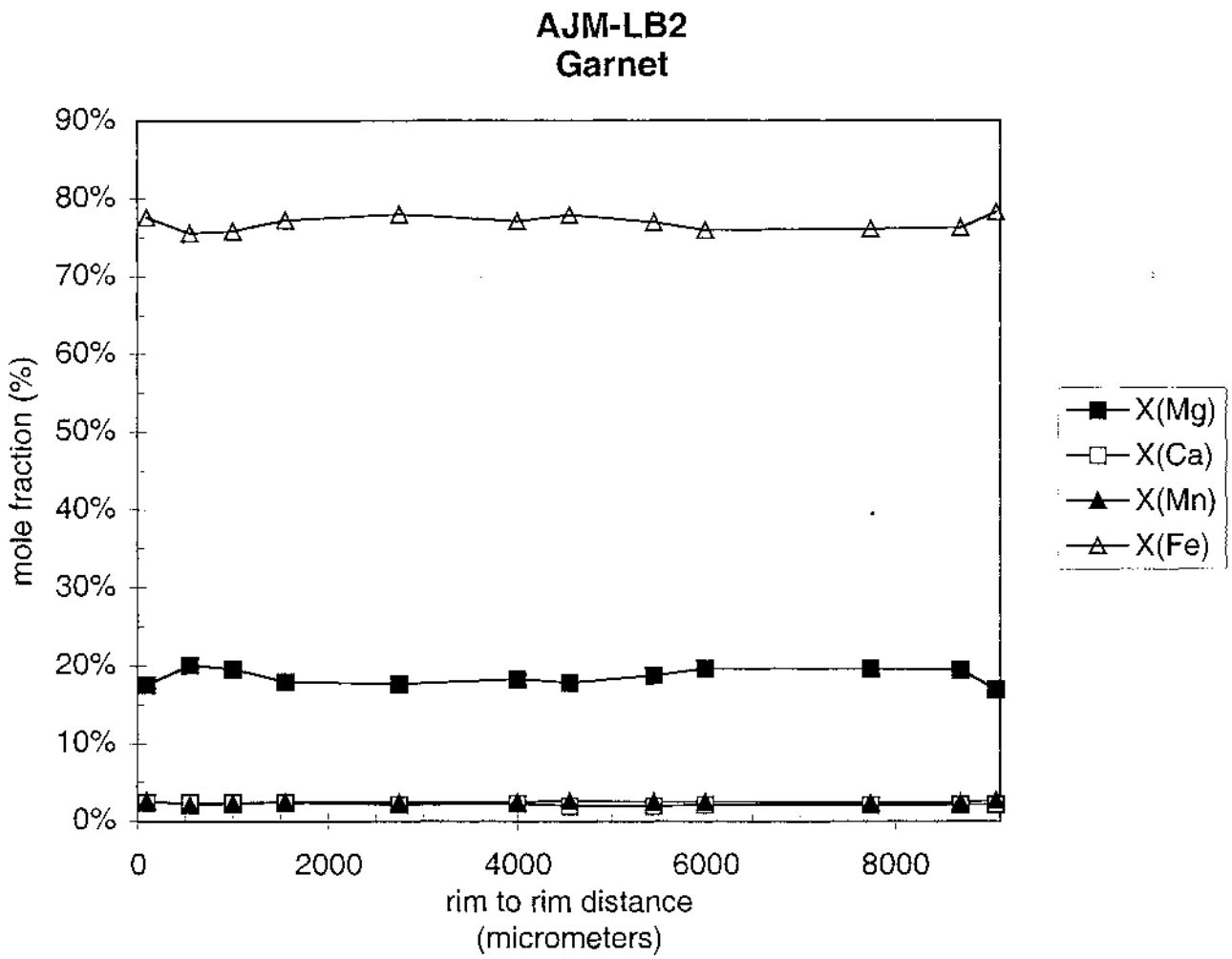
AJM-LB2
Garnet
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
mole fraction (%)
0
2000
4000
6000
8000
rim to rim distance
(micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR12

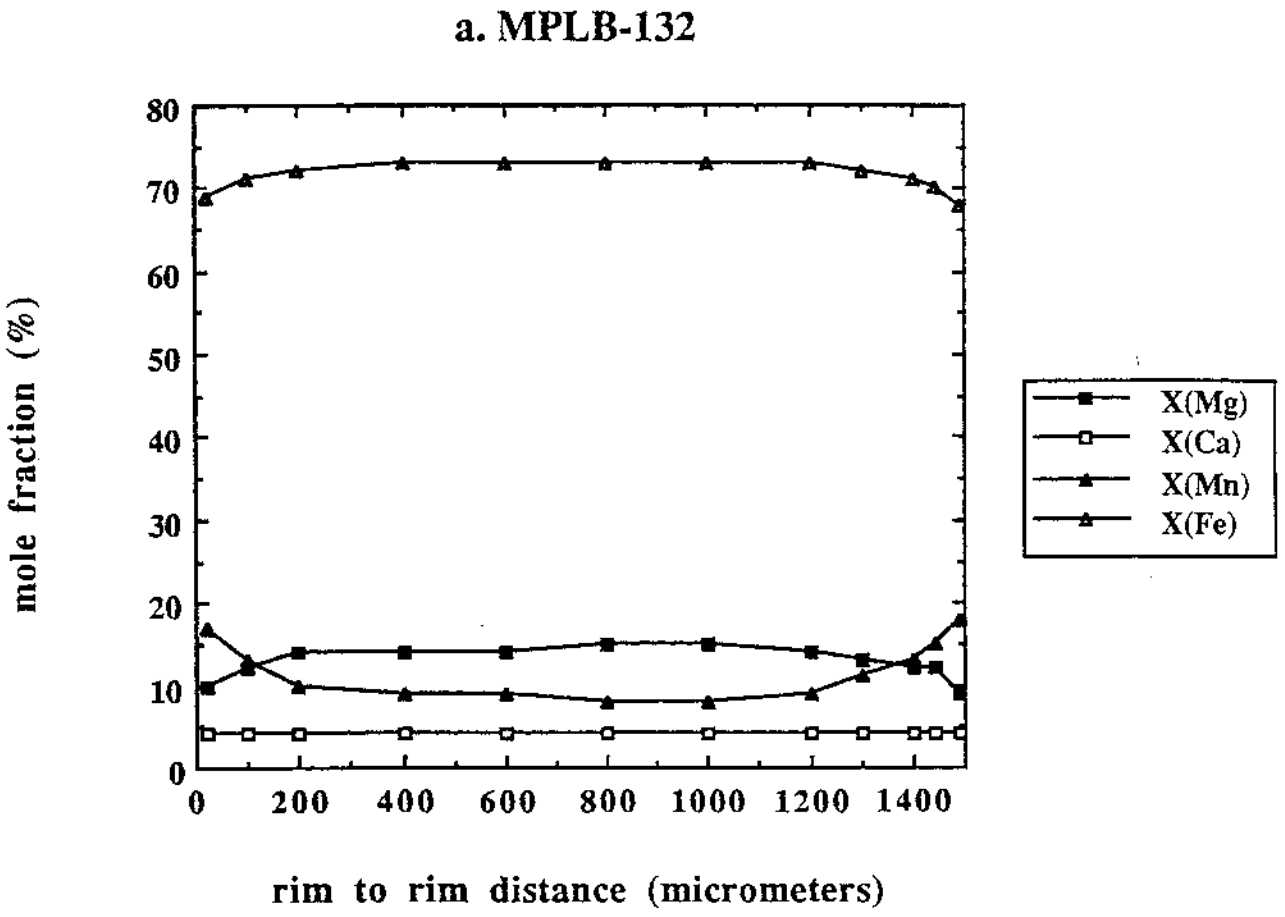
a. MPLB-132
mole fraction (%)
80
70
60
50
40
30
20
10
0
0
200
400
600
800
1000
1200
1400
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR13

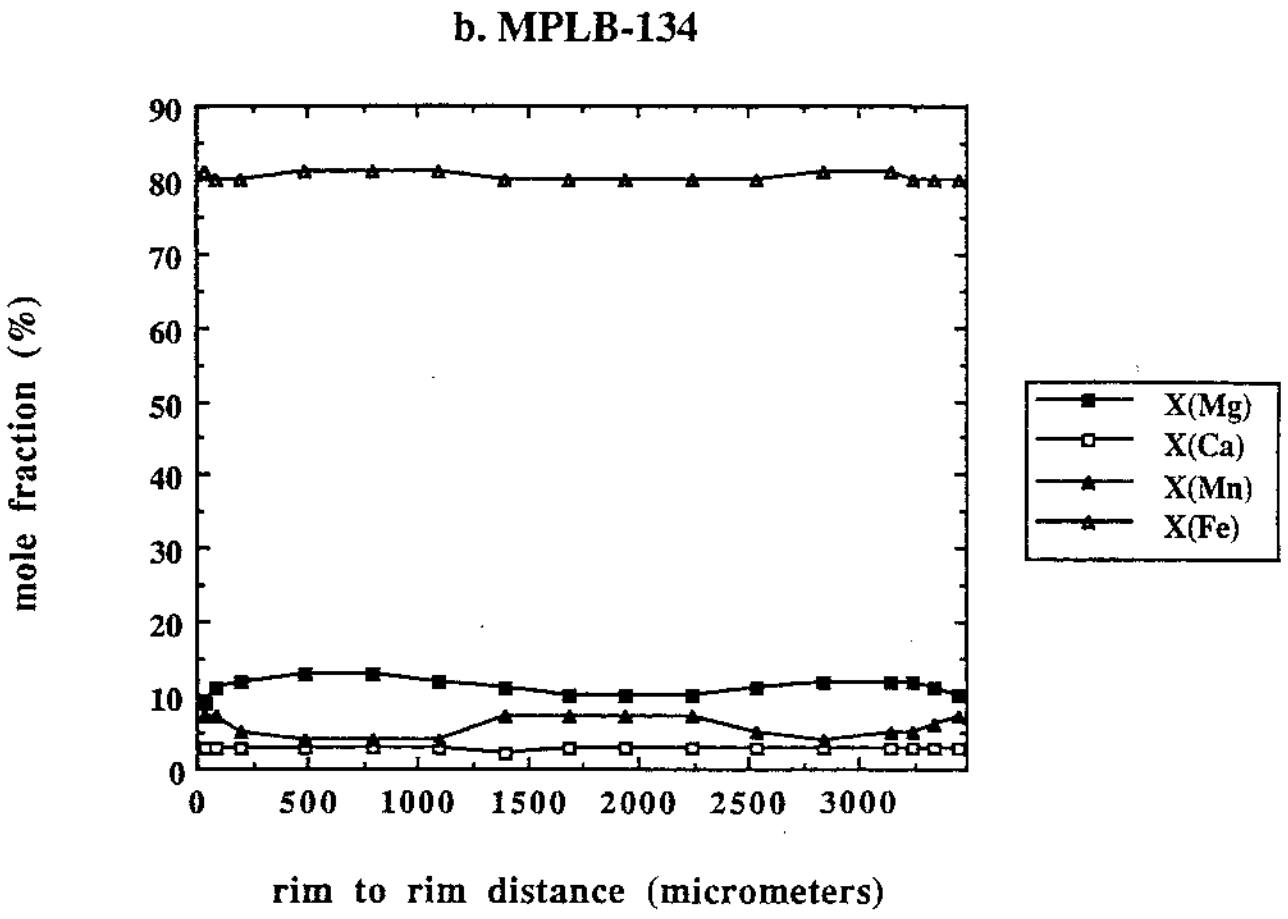
b. MPLB-134
mole fraction (%)
90
80
70
60
50
40
30
20
10
0
0
500
1000
1500
2000
2500
3000
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR14

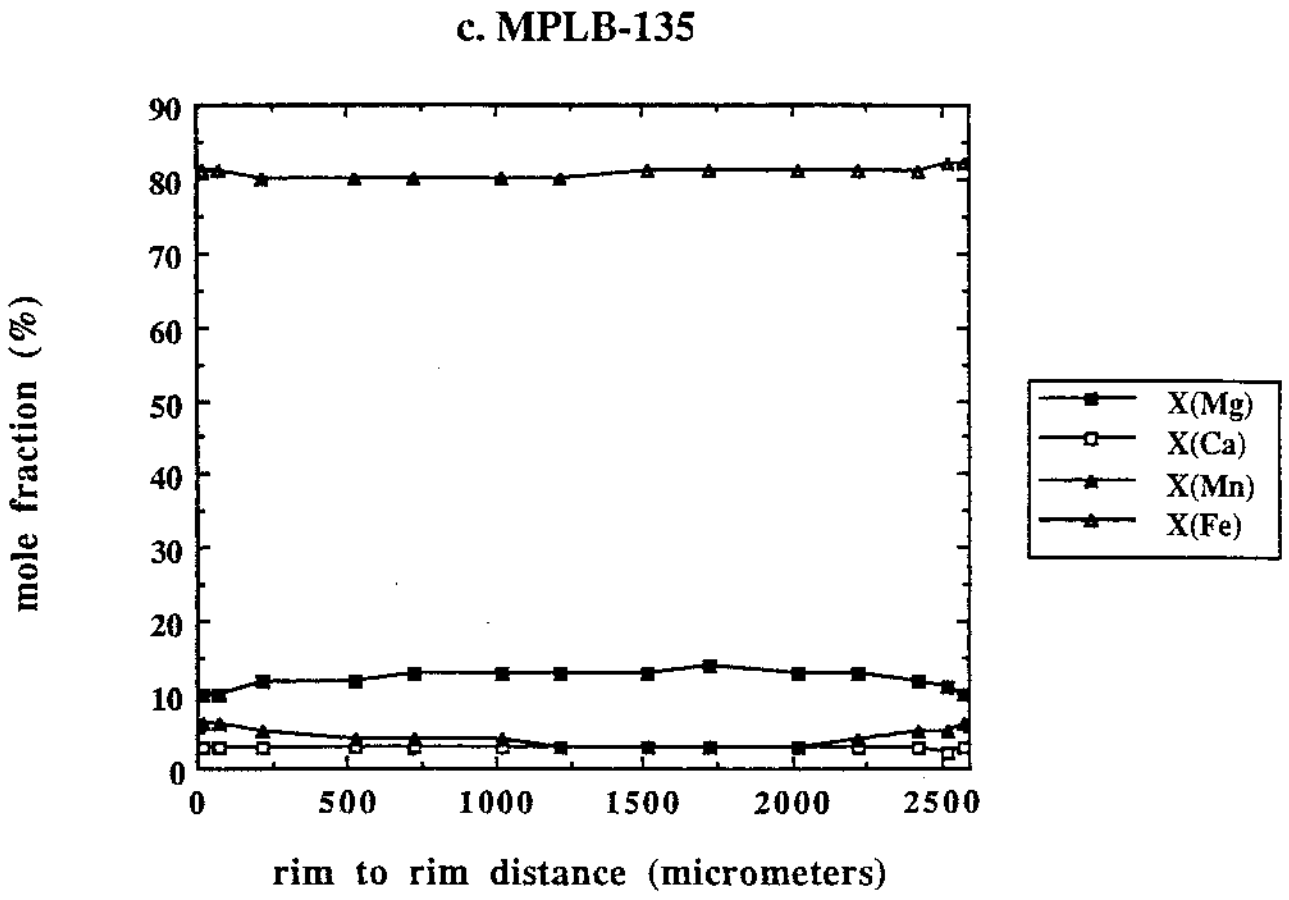
c. MPLB-135
mole fraction (%)
90
80
70
60
50
40
30
20
10
0
0
500
1000
1500
2000
2500
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR15

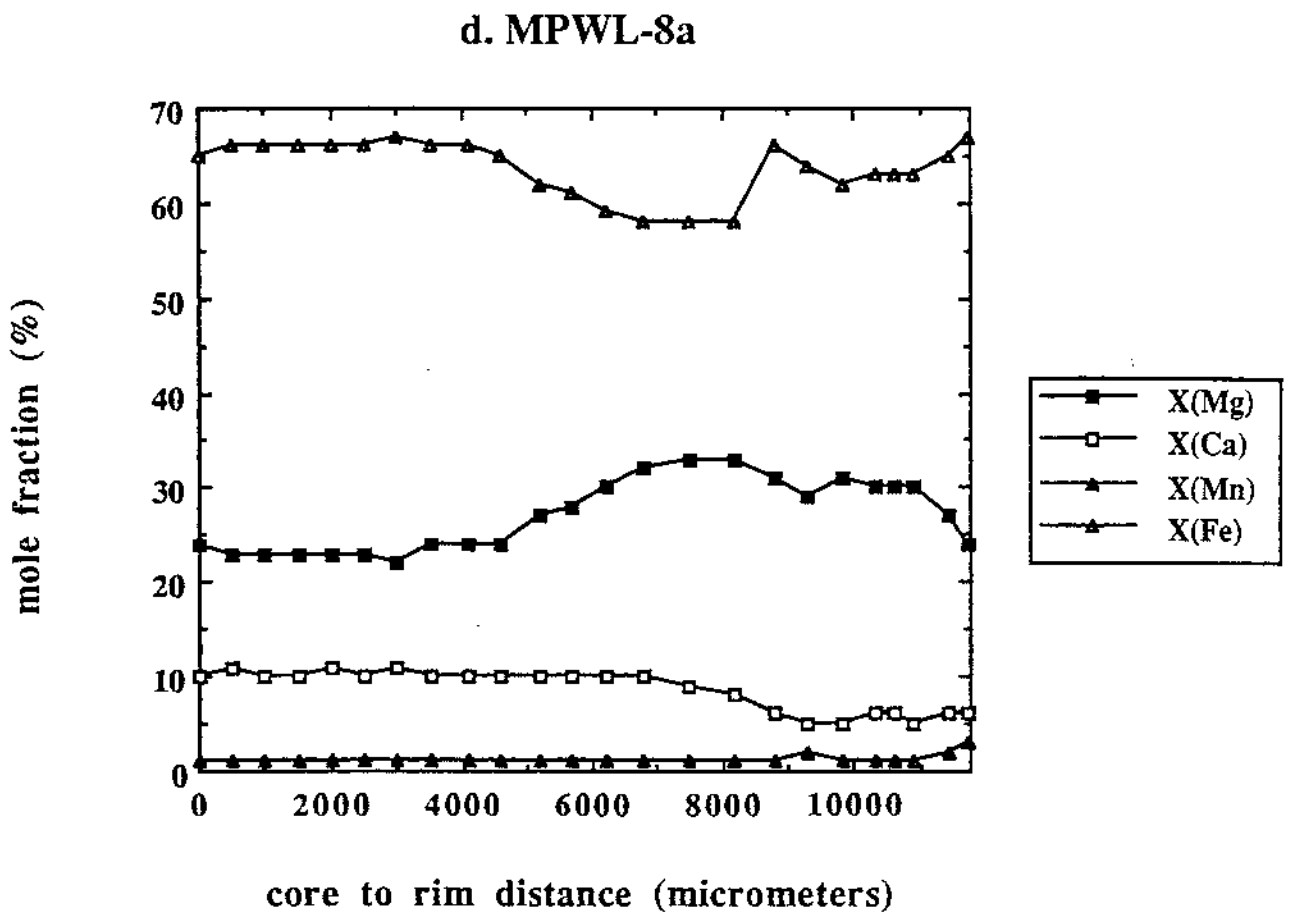
d. MPWL-8a
mole fraction (%)
70
60
50
40
30
20
10
0
0
2000
4000
6000
8000
10000
core to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR16

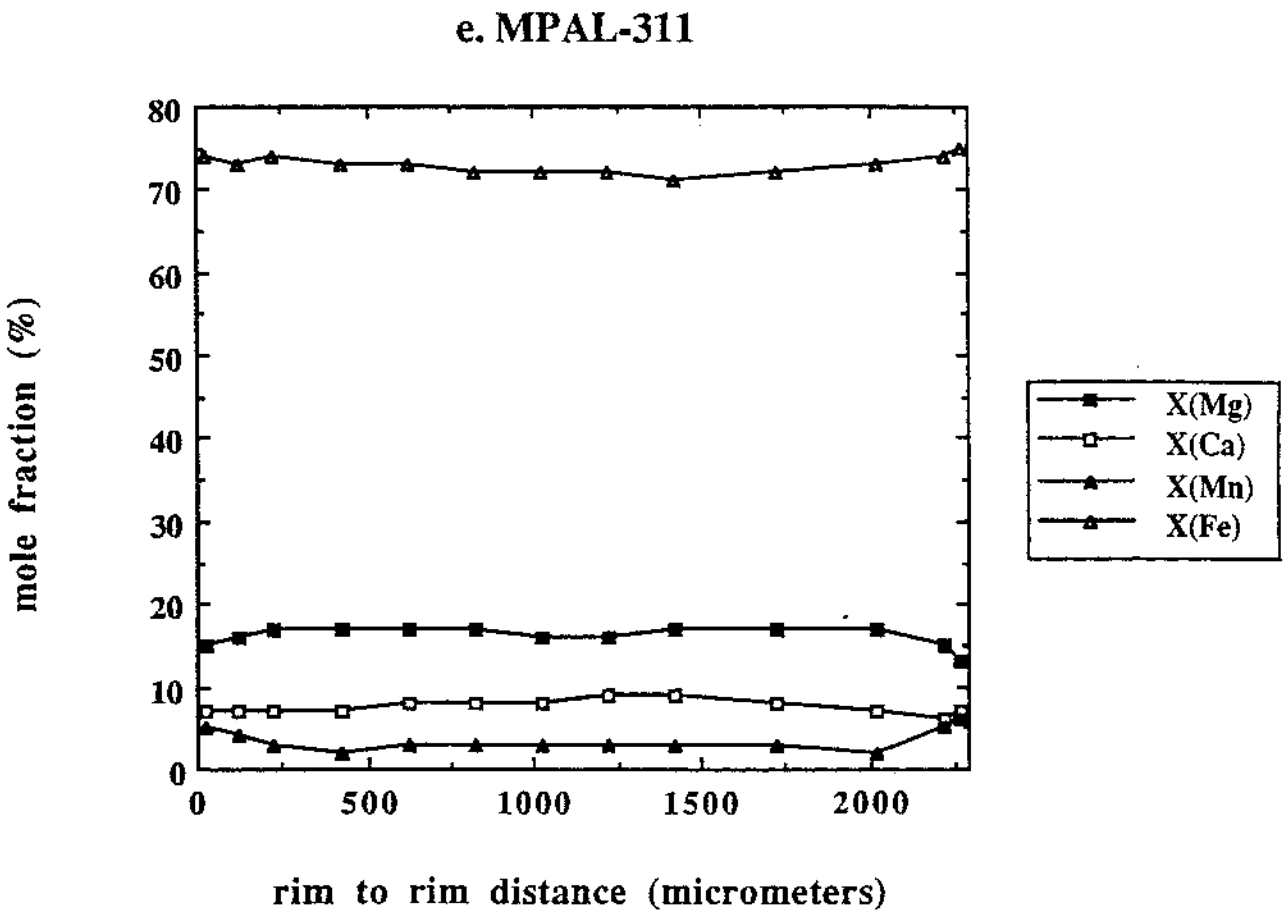
e. MPAL-311
mole fraction (%)
80
70
60
50
40
30
20
10
0
0
500
1000
1500
2000
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR17

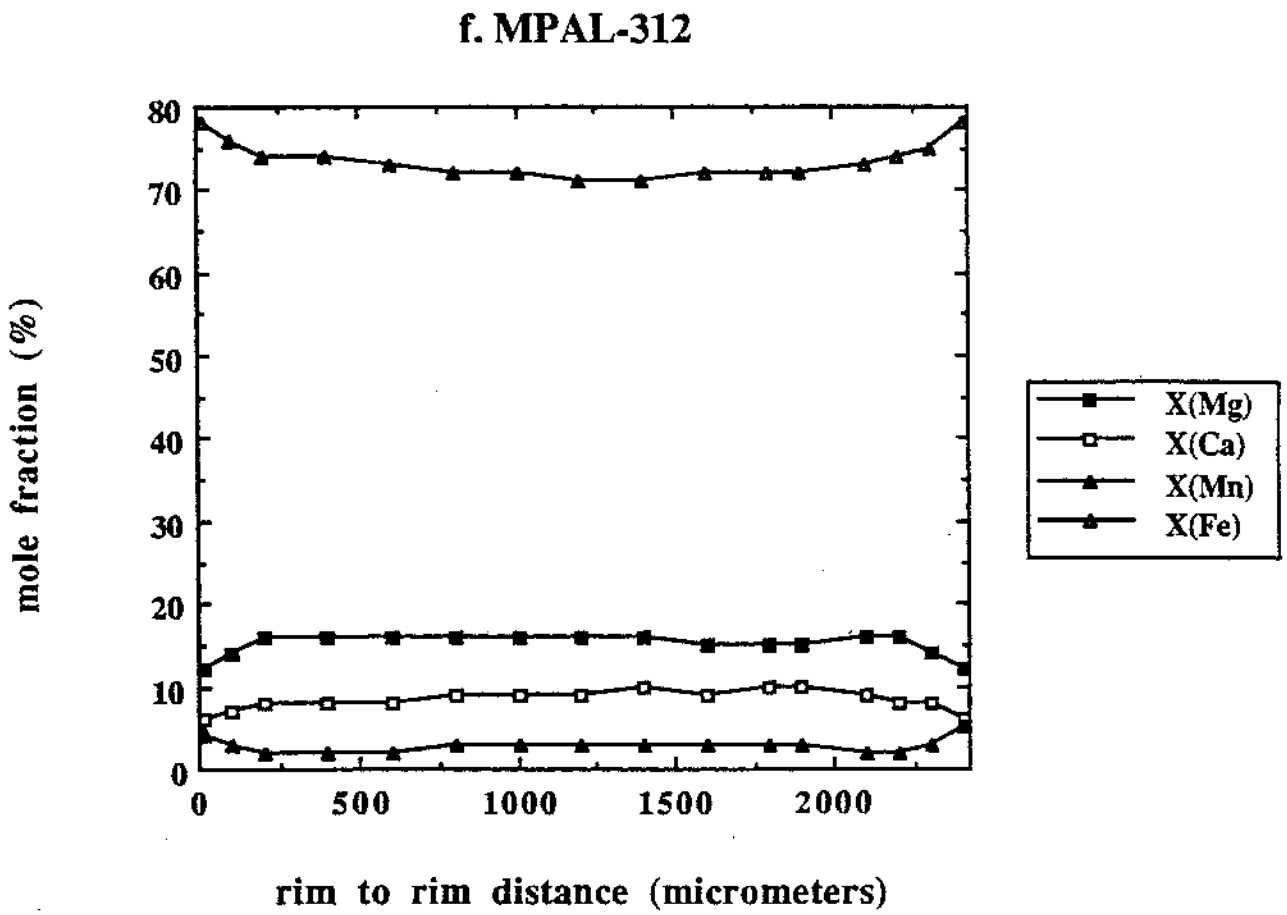
f. MPAL-312
mole fraction (%)
80
70
60
50
40
30
20
10
0
0
500
1000
1500
2000
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR18

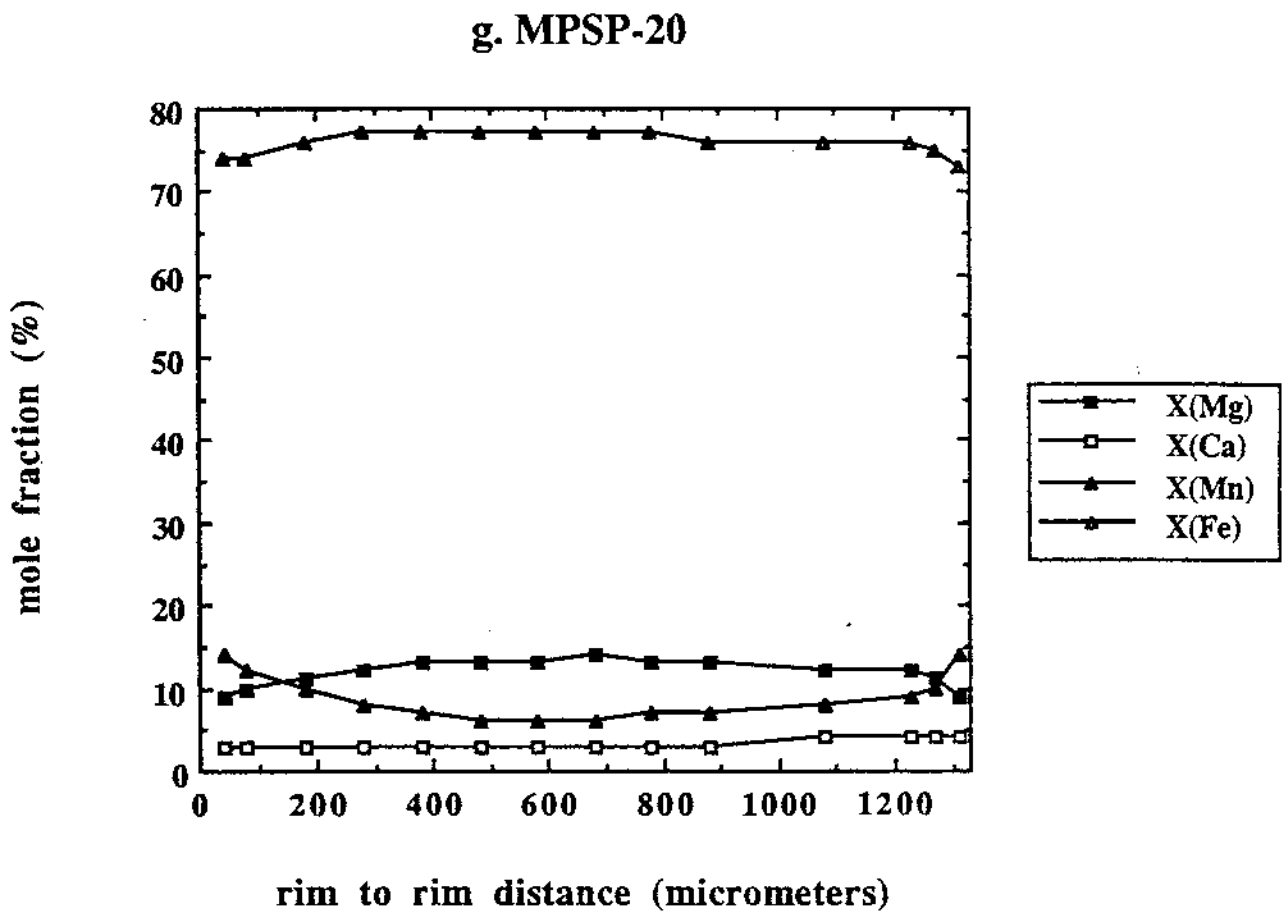
g. MPSP-20
mole fraction (%)
80
70
60
50
40
30
20
10
0
0
200
400
600
800
1000
1200
rim to rim distance (micrometers)
X(Mg)
X(Ca)
X(Mn)
X(Fe)

Figure DR19A

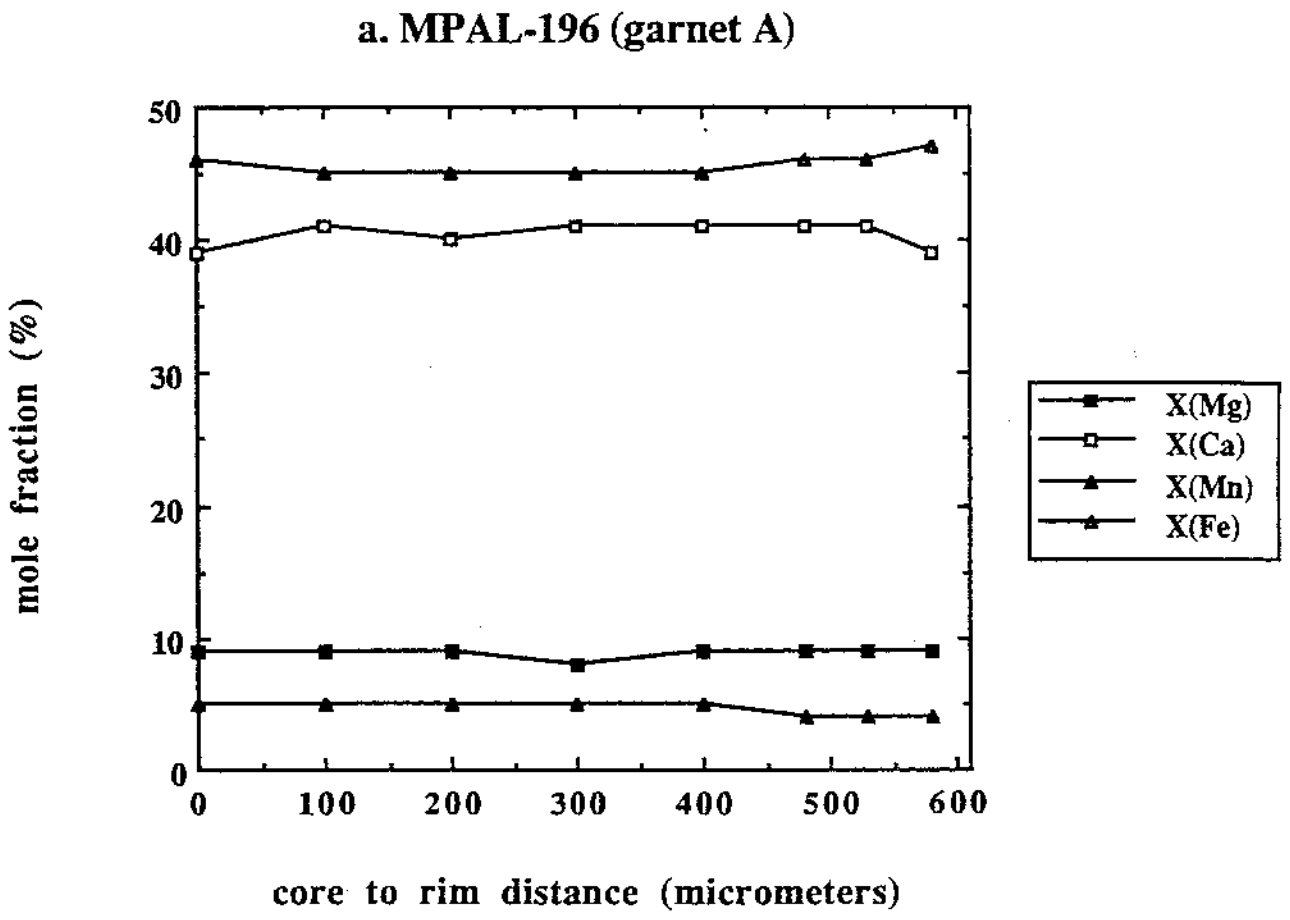
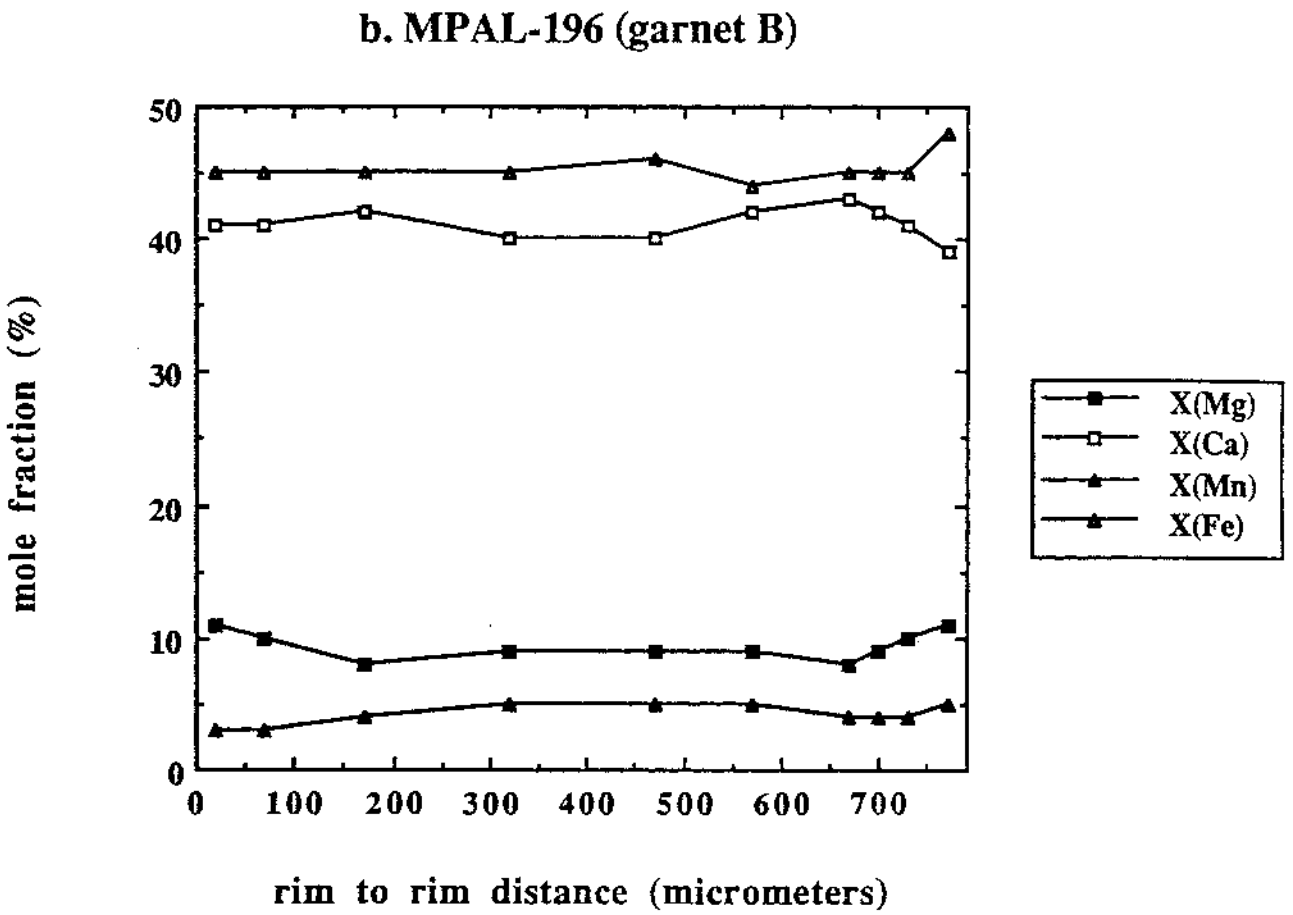
Figure DR19B