

Supplementary Table 2

Experimental data of Patino Douce et al. (1993, 1998), used to extract enthalpy of formation values for the Ti-biotite and member bio of this study (see text and Tab. 3).

The experimental data of Vielzeuf and Montel (1994) and Patino Douce and Bird (1995), as well as the natural data of Williams and Grambling 1990 and Holdaway et al. 1997 are also listed.

For reasons discussed in the text, these data are only used in the models of Fig. 1, 4 and 5, but not for extraction purposes.
People: X-calculation biotite, asmet and inerritic compositions are given for comparison. asmetline the biotite activity models Bio(D) and its ideal Fe-Mg mixture version Bio(Di) of this study, and models Bio(W) and Bio(TCC).
published by White et al. (2014) and Tajcmanova et al. (2020) for biotite, GSW for garnet (White et al. 2014) and EMP(W) for inerrite (White et al. 2020).

Bulk-compositions used in Pexler calculations are given in Supplementary Table 1 of this study. G22-compositions of the QFM buffer were simulated in the Pexler calculations.

Experimental data of Patino Douce et al. (1993, 1998): biotite-bearing experiments (Tab. 1), used for extracting H° [J/mol] of this study.

run	kbar	T °C	activity model	biotite										garnet					Bismette				
				experimental and computed composition: x_{Bi} (atoms per formula unit - 11 oxygens)										x_{Bi} (12 oxygens)					x_{Bi} (3 oxygens)				
				Si	Al (IV)	Al (IV)	Al (IV)	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	Ti	Mg	Mn	Fe ²⁺	Fe ³⁺	
				Si	Al (IV)	Al (IV)	Al (IV)	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	
APD-25	7	825	P093	2.656	1.304	0.417	0.073	0.202	1.222	0.568	0.940	0.888	0.543	0.198	0.705	0.034	0.027	0.037	0.987	0.044	0.008	0.958	0.014
			Bio(D)	2.640	1.360	0.466	0.083	0.216	1.154	0.018	1.01	0.959	0.512	0.317	0.623	0.030	0.027	0.013	0.961	0.099	0.006	0.855	0.079
			Bio(Di)	2.627	1.373	0.481	0.083	0.244	1.183	0.016	1.032	0.944	0.534	0.276	0.652	0.038	0.021	0.014	0.959	0.082	0.008	0.813	0.082
			Bio(W)	2.640	1.351	0.460	0.083	0.250	1.194	0.016	1.137	0.948	0.490	0.237	0.610	0.024	0.023	0.013	0.960	0.105	0.006	0.849	0.080
			Bio(TCC)	2.480	1.520	0.484		0.291	1.229	0.036	0.956	1.000	0.562	0.206	0.706	0.043	0.031	0.014	not stable				
APD-22	7	850	P093	2.690	1.310	0.352	0.042	0.222	1.153	0.000	1.064	0.877	0.530	0.213	0.720	0.028	0.027	0.012	0.973	0.060	0.005	0.909	0.040
			Bio(D)	2.676	1.324	0.431	0.082	0.237	0.976	0.016	1.297	0.959	0.430	0.361	0.591	0.021	0.014	0.013	0.956	0.114	0.006	0.837	0.077
			Bio(Di)	2.690	1.345	0.456	0.085	0.276	0.976	0.047	1.408	0.969	0.348	0.409	0.532	0.010	0.007	0.042	0.975	0.121	0.001	0.854	0.028
			Bio(W)	2.705	1.295	0.255		0.250	0.896	0.041	1.557	1.000	0.365	0.352	0.599	0.022	0.014	0.013	0.961	0.110	0.006	0.845	0.079
			Bio(TCC)	2.482	1.518	0.483		0.320	1.148	0.035	1.011	1.000	0.532	0.237	0.684	0.040	0.024	0.015	0.955	0.071	0.009	0.875	0.091
APD-33	7	875	P093	2.693	1.307	0.325	0.018	0.254	1.048	0.035	1.103	0.877	0.487	0.261	0.688	0.016	0.010	0.025	0.973	0.072	0.002	0.900	0.040
			Bio(TCC)	2.485	1.515	0.480		0.320	1.111	0.035	1.047	1.000	0.555	0.307	0.635	0.027	0.018	0.015	0.957	0.105	0.007	0.845	0.086
APD-34	7	900	P093	2.673	1.327	0.296	-0.031	0.256	0.963	0.059	1.196	0.897	0.446	0.292	0.647	0.014	0.008	0.039	0.971	0.087	0.002	0.884	0.041
			Bio(TCC)	2.497	1.503	0.470	0.000	0.315	0.924	0.032	1.219	1.000	0.421	0.255	0.598	0.020	0.014	0.015	0.960	0.120	0.006	0.834	0.096
APD-35	7	925	P093	2.661	1.339	0.282	-0.057	0.234	0.775	0.047	1.446	0.892	0.349	0.375	0.581	0.007	0.003	0.035	0.974	0.139	0.002	0.835	0.030
			Bio(W)	2.646	1.354	0.199	-0.155	0.346	0.740	0.052	1.388	0.909	0.348	0.409	0.532	0.010	0.007	0.042	0.975	0.121	0.001	0.854	0.028
APD-12	10	825	P093	2.657	1.343	0.401	0.178	0.225	1.231	0.056	0.944	0.884	0.565	0.158	0.695	0.043	0.028	0.014	0.971	0.048	0.007	0.922	0.046
			Bio(W)	2.678	1.282	0.463	0.181	0.208	1.096	0.009	0.964	0.873	0.532	0.201	0.721	0.041	0.025	0.013	0.975	0.055	0.003	0.915	0.041
APD-11	10	850	P093	2.679	1.271	0.401	0.080	0.249	1.037	0.026	1.021	0.882	0.504	0.252	0.697	0.021	0.011	0.019	0.967	0.087	0.003	0.896	0.055
			Bio(W)	2.682	1.285	0.355	-0.033	0.255	0.902	0.031	1.151	0.852	0.451	0.272	0.666	0.024	0.017	0.020	0.961	0.094	0.001	0.871	0.051
APD-4	10	900	P093	2.690	1.310	0.393	0.083	0.255	0.909	0.031	1.151	0.882	0.451	0.272	0.666	0.024	0.017	0.020	0.961	0.094	0.001	0.871	0.051

Experimental data of Vielzeuf and Montel (1994), analysis in Montel and Vielzeuf (1997).

run	kbar	°C	activity model	Si	Al (IV)	Al (IV)	Al (IV)	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	Ti	Mg	Mn	Fe ²⁺	Fe ³⁺
A117C	5	809		2.676	1.024	0.446	0.422	0.189	0.831	0.000	1.166		0.299	0.593	0.040	0.068		1.000	0.000	0.000	1.000	0.000
A117B	5	867		2.613	1.087	0.370	0.283	0.267	0.818	0.000	1.176		0.394	0.523	0.045	0.038		1.000	0.000	0.000	1.000	0.000
A118B	8	884		2.850	1.170	0.260	0.095	0.276	0.447	0.000	1.498		0.364	0.606	0.014	0.016		1.000	0.000	0.000	1.000	0.000
A119C	8	875		2.676	1.133	0.347	0.214	0.206	0.760	0.000	1.402		0.401	0.512	0.067	0.020		1.000	0.000	0.000	1.000	0.000
A119A	8	913		2.826	1.174	0.311	0.178	0.225	0.459	0.000	1.634		0.387	0.570	0.021	0.013		1.000	0.000	0.000	1.000	0.000
A119B	8	913		2.803	1.197	0.248	0.051	0.270	0.751	0.000	1.467		0.464	0.475	0.033	0.028		1.000	0.000	0.000	1.000	0.000
A114B	10	885		2.816	1.184	0.232	0.048	0.267	0.875	0.000	1.358		0.361	0.550	0.077	0.012		1.000	0.000	0.000	1.000	0.000

Experimental data of Patino Douce and Bird (1995)

run	kbar	°C	activity model	Si	Al (IV)	Al (IV)	Al (IV)	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	Ti	Mg	Mn	Fe ²⁺	Fe ³⁺
APD-88B	12.5	930		2.777	1.223	0.135		0.371	0.902	0.000	1.299		0.258	0.512	0.194	0.036		0.928	0.000	0.000	0.775	0.000
APD-89B	12.5	900		2.747	1.263	0.094		0.411	0.803	0.000	1.387		0.219	0.508	0.181	0.018		0.928	0.000	0.000	0.775	0.000
APD-91B	15	925		2.734	1.266	0.155		0.339	1.064	0.000	1.188		0.255	0.531	0.188	0.046		0.973	0.000	0.000	0.873	0.000
APD-94B	15	900		2.808	1.192	0.176		0.400	0.795	0.000	1.326		0.693	0.500	0.167	0.026		0.973	0.000	0.000	0.873	0.000
APD-97B	15	900		2.807	1.193	0.200		0.375	0.811	0.000	1.354		0.283	0.474	0.205	0.028		0.973	0.000	0.000	0.873	0.000

Natural data of Williams and Grambling (1990)

run	kbar	°C	activity model	Si	Al (IV)	Al (IV)	Al (IV)	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	X _{Fe}	Ti	Mg	Mn	Fe ²⁺	Fe ³⁺
77-85B	3.8	518		2.624	1.376	0.461	0.085	0.091	1.331	0.181	0.762		0.070	0.894	0.033	0.003		1.000	0.000	0.000	1.000	0.000
78-42D	3.8	502		2.633	1.367	0.461	0.084	0.090	1.297	0.179	0.889		0.086	0.886	0.025	0.003		0.980	0.000	0.010	0.970	0.040
77-81E	3.8	527		2.627	1.375	0.457	0.084	0.091	1.373	0.180	0.831		0.077	0.890	0.033	0.020		0.970	0.000	0.000	0.970	0.060
77-41	3.8	482		2.676	1.324	0.473	0.149	0.078	1.175	0.176	0.934		0.053	0.857	0.010	0.000		1.000	0.000	0.000	1.000	0.000
84-22A	3.8	504		2.606	1.394	0.466	0.074	0.086	1.406	0.191	0.680		0.081	0.814	0.025	0.080		1.000	0.000	0.000	0.980	0.020
77-73	3.8	493		2.634	1.366	0.422	0.056	0.092	1.186	0.193	0.995		0.038	0.842	0.033	0.087		0.990	0.000	0.130	0.862	0.120
77-73	3.8	484		2.603	1.397	0.458	0.061	0.088	1.438	0.273	0.586		0.062	0.802	0.032	0.104		1.000	0.000	0.000	0.980	0.020
83-45	3.8	487		2.656	1.344	0.456	0.112	0.091	1.228	0.200	0.841		0.117	0.634	0.052	0.197		0.820	0.000	0.030	0.790	0.360
77-46D	3.8	521		2.687	1.313	0.390	0.077	0.076	0.819	0.192	1.344		0.081	0.893	0.016	0.010		0.984	0.000	0.001	0.983	0.032
77-437	3.8	523		2.657	1.343	0.461	0.081	0.085	1.231	0.186	0.944		0.080	0.884	0.016	0.010		0.991	0.000	0.005	0.986	0.018
80-48	4.5	551		2.630	1.370	0.470	0.100	0.120	1.300	0.180	0.760		0.087	0.785	0.021	0.020		1.000	0.000	0.000	0.980	0.020
80-30	4.5	563		2.570	1.430	0.420	0.000	0.130	1.270	0.190	0.830		0.069	0.896	0.016	0.021		1.000	0.000	0.000	0.960	0.040
80-187	4.5	522		2.600	1.350	0.460	0.000	0.100	1.300	0.180	0.830		0.087	0.886	0.016	0.021		1.000	0.000	0.000	0.980	0.020
80-180	4.5	581		2.600	1.400	0.420	0.000	0.120	1.300	0.210	0.650		0.069	0.896	0.016	0.021		0.972	0.000	0.067	0.956	0.056
83-225	4.5	554		2.720	1.280	0.300	0.020	0.070	0.730	0.140	0.960		0.218	0.678	0.066	0.038		0.891	0.000	0.218	0.883	0.245
80-192D	4.5	562		2.700	1.330	0.450	0.020	0.070	0.730	0.140	0.960		0.218	0.678	0.066	0.038		0.891	0.000	0.218	0.883	0.245
81-234	4.5	585		2.740	1.260	0.360	0.000	0.080	0.810	0.150	1.430		0.183	0.687	0.062	0.068		0.877	0.000	0.138	0.859	0.246
80-148	4.5	588		2.760	1.260	0.410	0.020	0.080	0.810	0.150	1.430		0.183	0.687	0.062	0.068		0.877	0.000	0.138	0.859	0.246
CR-105	4.5	564		2.640	1.360	0.350	0.000	0.140	1.210	0.210	0.930		0.074	0.722	0.083	0.121		0.934	0.000	0.071	0.863	0.134
WB-303A	5	634		2.665	1.335	0.537	0.022	0.089	1.020	0.194	1.175		0.165	0.773	0.049	0.013		0.940	0.000	0.030	0.920	0.120
WB-303B	5	725		2.775	1.245	0.487	0.000	0.140	1.140	0.210	1.085		0.165	0.773	0.049	0.013		0.890	0.000	0.030	0.880	0.180
WB-94	5	489		2.664	1.366	0.366	0.000	0.089	1.144	0.202	1.012		0.067	0.740	0.068	0.125		0.910	0.000	0.030	0.890	0.180
WB-130	5	525		2.671	1.329	0.371	0.042	0.086	0.982	0.187	1.173		0.082	0.678	0.064	0.136		0.850	0.000	0.030	0.840	0.280
WB-140	5	525		2.671	1.329	0.382	0.088	0.082	0.982	0.187	1.173		0.082	0.678	0.064	0.136		0.850	0.000	0.030	0.840	0.280