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Fluid fugacities and phase equilibria in the Fe-Si-O-H-S system

Pingfang Shi

For deposit: Appendixes 1 and 2

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Appendix 1.

Thermal Expansions and Bulk Modulus of Some Solid Phases in the Fe-Si-O-H-S System.

No.	Name	α_0 (10^4)	α_1 (10^8)	α_2	K_0 (Mb)	$K_T'(P)$	$K_T'(T)$ (Mb/K)
1.	Quartz	0.31000	2.67800	0.00000	0.3740	6.40	0.00
2.	Iron	0.23987	2.56900	0.00000	1.6400	5.00	0.50
3.	Fayalite	0.26600	0.87360	- 0.24870	1.3657	5.16	- 0.258
4.	Clinoferrosilte	0.22160	0.00000	0.00000	1.0000	4.20	0.00
5.	Magnetite	0.26110	3.26020	0.00400	1.8300	4.00	0.00
6.	Hematite	0.24530	1.67020	0.00200	2.0700	4.53	0.00
7.	Wüstite (1)	0.16880	0.20400	0.01900	1.8000	4.00	0.40
8.	Wüstite (1.5)	0.24530	1.67020	0.00200	1.8000	4.00	0.40
9.	Pyrrhotite	0.97516	0.18936	0.00000	0.8330	4.00	0.00
10.	Pyrite	0.27186	1.54270	- 0.00359	1.4490	4.00	0.00
11.	$FeSO_4$	0.00000	0.00000	0.00000	1.0000	4.00	0.00

Expression for thermal expansion: $\alpha(T) = \alpha_0 + \alpha_1 T + \alpha_2 T^{-2}$

Data Sources for thermal expansion $\alpha(T)$ *and bulk modulus* $K_T(P,T)$*:*

1. $\alpha(T)$, Skinner (1966); $K_T(P,T)$, Soga (1968).
2. $\alpha(T)$, Guillermet and Gustafson (1985); $K_T(P,T)$, Mao et al. (1967).
3. $\alpha(T)$, Suzuki et al. (1981); $K_T(P,T)$, Sumino (1979).
4. $\alpha(T)$, Skinner (1966); $K_T(P,T)$, Akimoto (1972)
5. $\alpha(T)$, Haas (1988); $K_T(P,T)$, Mao et al. (1974).
6. $\alpha(T)$, Haas (1988); $K_T(P,T)$, Liebermann and Schreiber (1968).

7, 8. $\alpha(T)$ and $K_T(P,T)$, Fei and Saxena (1986).

9, 10. $\alpha(T)$ and $K_T(P,T)$, assessed in this study [based on data from Scott (1973)].

11. $\alpha(T)$ and $K_T(P,T)$, estimated in this study.

Appendix 2.

The Log f_{O_2}- Log f_{H_2}-T- P Relations of Some Oxygen Buffers in the Fe-Si-O-H System.

1. Hm-Mt Buffer;
2. Fay-Qtz-Mt Buffer;
3. Fay-Qtz-Fe Buffer;
4. Mt-Fe Buffer;
5. Wüs-Fe Buffer;
6. Wüs-Mt Buffer.

1a. Log f_{O_2}- T - P Relations of Hm-Mt f_{O_2} Buffer

	P (bar)					
T(°C)	1	1000	2000	4000	5000	10000
200.0	-39.992	-40.138	-40.333	-40.732	-40.930	-41.792
250.0	-34.774	-34.917	-35.090	-35.461	-35.642	-36.424
300.0	-30.456	-30.596	-30.762	-31.098	-31.265	-31.981
350.0	-26.818	-26.955	-27.108	-27.420	-27.575	-28.236
400.0	-23.705	-23.837	-23.981	-24.272	-24.417	-25.031
450.0	-21.004	-21.132	-21.268	-21.541	-21.676	-22.251
500.0	-18.633	-18.758	-18.884	-19.143	-19.270	-19.810
550.0	-16.530	-16.650	-16.772	-17.015	-17.136	-17.645
600.0	-14.637	-14.754	-14.870	-15.101	-15.215	-15.698
650.0	-12.938	-13.051	-13.161	-13.382	-13.491	-13.949
700.0	-11.427	-11.537	-11.642	-11.853	-11.957	-12.394
750.0	-10.083	-10.189	-10.291	-10.493	-10.593	-11.010
800.0	-8.873	-8.976	-9.074	-9.268	-9.364	-9.764
850.0	-7.778	-7.878	-7.972	-8.159	-8.251	-8.635
900.0	-6.780	-6.877	-6.968	-7.149	-7.238	-7.607
950.0	-5.868	-5.962	-6.050	-6.225	-6.311	-6.667
1000.0	-5.031	-5.123	-5.208	-5.377	-5.461	-5.804
1050.0	-4.258	-4.347	-4.430	-4.595	-4.675	-5.007
1100.0	-3.541	-3.628	-3.709	-3.869	-3.947	-4.268
1150.0	-2.875	-2.961	-3.040	-3.194	-3.270	-3.582
1200.0	-2.255	-2.337	-2.415	-2.566	-2.641	-2.944
1250.0	-1.678	-1.763	-1.834	-1.982	-2.055	-2.349
1300.0	-1.204	-1.220	-1.293	-1.439	-1.509	-1.796
1350.0	-0.641	-0.723	-0.795	-0.932	-1.002	-1.281
1400.0	-0.176	-0.251	-0.322	-0.462	-0.530	-0.802

1b. Log f_{H_2}- T - P Relations of Hm-Mt-Water Assemblage

	P (bar)					
T(°C)	1	1000	2000	4000	5000	10000
200.0	-4.334	-3.141	-3.117	-3.077	-3.030	-3.020
300.0	-4.402	-2.519	-2.472	-2.409	-2.389	-2.326
400.0	-4.462	-2.178	-2.105	-2.016	-1.992	-1.879
500.0	-4.531	-2.004	-1.902	-1.786	-1.750	-1.596
600.0	-4.621	-1.943	-1.811	-1.667	-1.617	-1.431
700.0	-4.705	-1.933	-1.771	-1.599	-1.538	-1.327
800.0	-4.742	-1.911	-1.718	-1.520	-1.450	-1.219
900.0	-4.757	-1.892	-1.669	-1.445	-1.368	-1.122
1000.0	-4.761	-1.876	-1.624	-1.376	-1.295	-1.036
1100.0	------	-1.868	-1.587	-1.317	-1.232	-0.964
1200.0		-1.865	-1.557	-1.266	-1.179	-0.903
1300.0		-1.864	-1.528	-1.219	-1.130	-0.847
1400.0		-1.858	-1.497	-1.172	-1.080	-0.792

2a. Log f_{O_2}- T - P Relations of Fay-Qtz-Mt f_{O_2} Buffer

	P (bar)					
T(°C)	1	1000	2000	4000	5000	10000
200.0	-46.072	-46.049	-46.076	-46.145	-46.180	-46.247
250.0	-40.538	-40.527	-40.552	-40.614	-40.645	-40.698
300.0	-35.993	-35.989	-36.012	-36.068	-36.096	-36.136
350.0	-32.202	-32.204	-32.225	-32.275	-32.300	-32.329
400.0	-29.001	-29.008	-29.027	-29.071	-29.094	-29.113
450.0	-26.272	-26.281	-26.299	-26.338	-26.358	-26.369
500.0	-23.926	-23.936	-23.952	-23.987	-24.004	-24.007
550.0	-21.894	-21.906	-21.919	-21.950	-21.965	-21.961
600.0	-20.130	-20.142	-20.154	-20.181	-20.194	-20.182
650.0	-18.584	-18.597	-18.607	-18.630	-18.642	-18.623
700.0	-17.213	-17.225	-17.234	-17.254	-17.263	-17.237
750.0	-15.986	-15.998	-16.005	-16.022	-16.029	-15.997
800.0	-14.881	-14.892	-14.898	-14.912	-14.918	-14.880
850.0	-13.880	-13.890	-13.895	-13.905	-13.910	-13.866
900.0	-12.968	-12.977	-12.981	-12.988	-12.991	-12.941
950.0	-12.133	-12.141	-12.143	-12.148	-12.150	-12.094
1000.0	-11.366	-11.373	-11.374	-11.376	-11.377	-11.315
1050.0	-10.658	-10.664	-10.664	-10.664	-10.663	-10.595
1100.0	-10.003	-10.008	-10.007	-10.004	-10.002	-9.929
1150.0	-9.396	-9.399	-9.397	-9.392	-9.388	-9.310
1200.0	-8.831	-8.833	-8.829	-8.822	-8.818	-8.734
1250.0	-8.305	-8.305	-8.301	-8.291	-8.286	-8.196
1300.0	-7.813	-7.813	-7.807	-7.796	-7.789	-7.694
1350.0	-7.355	-7.352	-7.346	-7.333	-7.325	-7.225
1400.0	-6.926	-6.922	-6.915	-6.899	-6.890	-6.785
1450.0	-6.524	-6.520	-6.511	-6.494	-6.484	-6.373
1500.0	-6.149	-6.143	-6.134	-6.114	-6.103	-5.987
1550.0	-5.797	-5.790	-5.780	-5.758	-5.746	-5.625
1600.0	-5.468	-5.459	-5.448	-5.425	-5.412	-5.286
1650.0	-5.160	-5.150	-5.138	-5.113	-5.099	-4.968
1700.0	-4.872	-4.860	-4.847	-4.820	-4.805	-4.669
1750.0	-4.602	-4.589	-4.576	-4.547	-4.531	-4.390
1800.0	-4.350	-4.336	-4.321	-4.291	-4.274	-4.128

2b. Log f_{H_2}- T - P Relations of Fay-Qtz-Mt-Water Assemblage

	P (bar)					
T(°C)	1	1000	2000	4000	5000	10000
200.0	-1.316	-0.186	-0.245	-0.371	-0.405	-0.792
300.0	-1.644	0.178	0.154	0.076	0.027	-0.248
400.0	-1.820	0.407	0.418	0.383	0.346	0.162
500.0	-1.890	0.585	0.631	0.636	0.617	0.503
600.0	-1.880	0.750	0.831	0.873	0.872	0.811
700.0	-1.819	0.909	1.024	1.101	1.115	1.095
800.0	-1.746	1.044	1.192	1.301	1.327	1.339
900.0	-1.673	1.154	1.334	1.473	1.508	1.545
1000.0	-1.604	1.242	1.454	1.620	1.661	1.718
1100.0	-1.541	1.314	1.556	1.747	1.792	1.865
1200.0	-1.484	1.373	1.643	1.856	1.905	1.990
1300.0	-1.430	1.422	1.719	1.952	2.004	2.099
1400.0	-1.379	1.466	1.787	2.038	2.093	2.196
1500.0	-1.328	1.506	1.852	2.116	2.175	2.284
1600.0	-1.276	1.546	1.913	2.188	2.253	2.367
1700.0	-1.222	1.586	1.974	2.257	2.328	2.446
1800.0	-1.165	1.629	2.035	2.323	2.404	2.524

3a. Log f_{O_2}- T - P Relations of Fay-Qtz-Fe f_{O_2} Buffer

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
200.0	-54.878	-54.923	-54.958	-55.087	-55.484	-56.009
250.0	-48.920	-48.966	-49.003	-49.121	-49.484	-49.957
300.0	-44.006	-44.053	-44.090	-44.199	-44.533	-44.964
350.0	-39.884	-39.930	-39.968	-40.070	-40.379	-40.774
400.0	-36.376	-36.421	-36.460	-36.555	-36.842	-37.207
450.0	-33.355	-33.399	-33.437	-33.527	-33.795	-34.134
500.0	-30.725	-30.768	-30.806	-30.890	-31.142	-31.457
550.0	-28.415	-28.456	-28.494	-28.573	-28.810	-29.105
600.0	-26.367	-26.406	-26.443	-26.518	-26.743	-27.020
650.0	-24.537	-24.575	-24.611	-24.683	-24.895	-25.156
700.0	-22.892	-22.928	-22.964	-23.032	-23.234	-23.480
750.0	-21.404	-21.439	-21.474	-21.539	-21.731	-21.963
800.0	-20.047	-20.081	-20.115	-20.177	-20.360	-20.580
850.0	-18.807	-18.839	-18.872	-18.932	-19.107	-19.315
900.0	-17.670	-17.701	-17.733	-17.791	-17.958	-18.156
950.0	-16.622	-16.653	-16.684	-16.739	-16.900	-17.088
1000.0	-15.657	-15.687	-15.717	-15.770	-15.924	-16.103
1050.0	-14.765	-14.794	-14.823	-14.874	-15.023	-15.193
1100.0	-13.938	-13.966	-13.994	-14.043	-14.187	-14.349
1150.0	-13.169	-13.197	-13.223	-13.271	-13.410	-13.564
1200.0	-12.453	-12.479	-12.505	-12.552	-12.685	-12.833
1250.0	-11.784	-11.809	-11.834	-11.879	-12.008	-12.149
1300.0	-11.157	-11.182	-11.205	-11.249	-11.375	-11.509
1350.0	-10.568	-10.593	-10.616	-10.658	-10.779	-10.918
1400.0	-10.015	-10.039	-10.060	-10.102	-10.220	-10.383

3b. Log f_{H_2}- T - P Relations of Fay-Qtz-Fe-Water Assemblage

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
200.0	-0.001	2.691	2.994	3.293	3.690	3.982
250.0	-0.001	2.691	2.992	3.291	3.686	3.976
300.0	-0.002	2.691	2.990	3.288	3.681	3.969
350.0	-0.003	2.690	2.987	3.285	3.675	3.962
400.0	-0.006	2.688	2.983	3.280	3.669	3.955
450.0	-0.009	2.684	2.979	3.275	3.661	3.947
500.0	-0.013	2.680	2.975	3.269	3.654	3.939
550.0	-0.018	2.674	2.969	3.263	3.646	3.931
600.0	-0.024	2.668	2.963	3.255	3.637	3.922
650.0	-0.031	2.660	2.956	3.247	3.629	3.913
700.0	-0.039	2.652	2.947	3.238	3.619	3.903
750.0	-0.048	2.642	2.938	3.229	3.610	3.893
800.0	-0.058	2.632	2.928	3.218	3.599	3.882
850.0	-0.069	2.622	2.916	3.206	3.588	3.871
900.0	-0.081	2.610	2.903	3.194	3.576	3.859
950.0	-0.094	2.599	2.888	3.180	3.564	3.846
1000.0	-0.107	2.588	2.873	3.167	3.552	3.834
1050.0	-0.121	2.578	2.857	3.153	3.541	3.822
1100.0	-0.135	2.568	2.840	3.139	3.529	3.810
1150.0	-0.149	2.559	2.822	3.125	3.518	3.798
1200.0	-0.163	2.550	2.804	3.112	3.507	3.787
1250.0	-0.177	2.543	2.786	3.098	3.496	3.776
1300.0	-0.191	2.536	2.767	3.084	3.486	3.765
1350.0	-0.205	2.530	2.748	3.071	3.475	3.757
1400.0	-0.219	2.525	2.729	3.058	3.465	3.754

4a. Log f_{O_2}- T - P Relations of Mt-Fe f_{O_2} Buffer

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
200.0	-52.677	-52.709	-52.731	-52.834	-53.158	-53.569
250.0	-46.824	-46.859	-46.884	-46.979	-47.274	-47.642
300.0	-42.002	-42.038	-42.065	-42.153	-42.424	-42.757
350.0	-37.963	-37.999	-38.027	-38.109	-38.359	-38.663
400.0	-34.532	-34.568	-34.597	-34.673	-34.905	-35.184
450.0	-31.584	-31.619	-31.648	-31.720	-31.936	-32.192
500.0	-29.025	-29.059	-29.089	-29.155	-29.357	-29.595
550.0	-26.785	-26.817	-26.847	-26.910	-------	-------
600.0	-------	-------	-------	-------		

4b. Log f_{H_2}- T - P Relations of Mt-Fe-Water Assemblage

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
200.0	-0.004	2.412	2.920	3.123	3.081	2.868
250.0	-0.010	2.579	2.910	3.169	3.140	2.973
300.0	-0.018	2.619	2.898	3.151	3.181	3.059
350.0	-0.030	2.623	2.883	3.131	3.208	3.130
400.0	-0.046	2.612	2.867	3.111	3.227	3.188
450.0	-0.065	2.594	2.850	3.091	3.240	3.238
500.0	-0.085	2.574	2.832	3.071	3.249	3.280
550.0	-0.106	2.553	2.815	3.053	------	------
600.0	------	------	------	------		

5a. Log f_{O_2}- T - P Relations of Wüs-Fe f_{O_2} Buffer

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
400.0						
450.0		Mt-Fe Buffer Range				
500.0					-------	-------
550.0	-------	-------	-------	-------	-27.109	-27.383
600.0	-24.824	-24.860	-24.895	-24.965	-25.174	-25.431
650.0	-23.113	-23.148	-23.182	-23.249	-23.447	-23.688
700.0	-21.577	-21.611	-21.644	-21.707	-21.896	-22.123
750.0	-20.189	-20.222	-20.254	-20.314	-20.493	-20.708
800.0	-18.924	-18.956	-18.987	-19.045	-19.216	-19.419
850.0	-17.769	-17.800	-17.830	-17.885	-18.049	-18.240
900.0	-16.712	-16.741	-16.771	-16.824	-16.980	-17.162
950.0	-15.738	-15.767	-15.796	-15.847	-15.996	-16.169
1000.0	-14.842	-14.870	-14.898	-14.947	-15.090	-15.254
1050.0	-14.015	-14.042	-14.069	-14.116	-14.254	-14.410
1100.0	-13.250	-13.276	-13.302	-13.347	-13.480	-13.628
1150.0	-12.540	-12.565	-12.589	-12.634	-12.762	-12.902
1200.0	-11.878	-11.903	-11.927	-11.969	-12.093	-12.226
1250.0	-11.262	-11.285	-11.308	-11.350	-11.469	-11.596
1300.0	-10.685	-10.708	-10.730	-10.770	-10.886	-11.006
1350.0	-10.145	-10.167	-10.188	-10.227	-10.339	-10.454
1400.0	-9.637	-9.659	-9.679	-9.717	-9.825	-9.934

5b. Log f_{H_2}- T - P Relations of Wüs-Fe-Water Assemblage

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
400.0						
450.0		Mt-Fe-Water Assemblage Range				
500.0					------	------
550.0	------	------	------	------	3.260	3.347
600.0	-0.126	2.535	2.804	3.047	3.289	3.405
650.0	-0.140	2.523	2.797	3.045	3.311	3.451
700.0	-0.154	2.512	2.790	3.042	3.326	3.489
750.0	-0.168	2.501	2.781	3.037	3.338	3.518
800.0	-0.182	2.489	2.770	3.031	3.345	3.540
850.0	-0.196	2.479	2.759	3.024	3.349	3.556
900.0	-0.209	2.470	2.747	3.016	3.352	3.569
950.0	-0.222	2.461	2.734	3.009	3.353	3.578
1000.0	-0.235	2.455	2.721	3.001	3.355	3.586
1050.0	-0.246	2.450	2.709	2.995	3.356	3.593
1100.0	-0.256	2.446	2.696	2.989	3.357	3.599
1150.0	-0.266	2.445	2.684	2.983	3.358	3.604
1200.0	-0.275	2.444	2.673	2.978	3.359	3.609
1250.0	-0.283	2.445	2.661	2.973	3.360	3.613
1300.0	-0.290	2.446	2.650	2.969	3.361	3.617
1350.0	-0.297	2.449	2.639	2.965	3.362	3.620
1400.0	-0.303	2.452	2.628	2.961	3.363	3.623

6a. Log f_{O_2}- T - P Relations of Wüs-Mt f_{O_2} Buffer

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
400.0						
450.0		Mt-Fe Buffer Range				
500.0					-------	-------
550.0	-------	-------	-------	-------	-27.070	-27.129
600.0	-24.758	-24.774	-24.788	-24.816	-24.900	-24.948
650.0	-22.855	-22.870	-22.883	-22.909	-22.986	-23.024
700.0	-21.157	-21.171	-21.184	-21.208	-21.277	-21.307
750.0	-19.630	-19.644	-19.657	-19.678	-19.741	-19.762
800.0	-18.249	-18.262	-18.274	-18.294	-18.351	-18.364
850.0	-16.992	-17.004	-17.016	-17.034	-17.085	-17.090
900.0	-15.842	-15.853	-15.865	-15.881	-15.927	-15.924
950.0	-14.786	-14.796	-14.806	-14.821	-14.862	-14.852
1000.0	-13.810	-13.820	-13.830	-13.843	-13.878	-13.862
1050.0	-12.907	-12.916	-12.925	-12.936	-12.968	-12.945
1100.0	-12.068	-12.076	-12.084	-12.094	-12.121	-12.092
1150.0	-11.286	-11.293	-11.300	-11.309	-11.332	-11.296
1200.0	-10.555	-10.562	-10.568	-10.576	-10.594	-10.552
1250.0	-9.871	-9.877	-9.882	-9.889	-9.903	-9.856
1300.0	-9.229	-9.235	-9.239	-9.244	-9.255	-9.201
1350.0	-8.626	-8.631	-8.635	-8.639	-8.646	-8.587
1400.0	-8.059	-8.063	-8.066	-8.069	-8.073	-8.008

6b. Log f_{H_2}- T - P Relations of Wüs-Mt-Water Assemblage

	P (bar)					
T(°C)	1	500	1000	2000	5000	10000
400.0						
450.0		Mt-Fe-Water Assemblage Range				
500.0					------	------
550.0	------	------	------	------	3.243	3.226
600.0	-0.135	2.521	2.782	3.006	3.174	3.177
650.0	-0.180	2.470	2.730	2.945	3.120	3.142
700.0	-0.229	2.418	2.678	2.889	3.074	3.112
750.0	-0.278	2.367	2.626	2.837	3.034	3.086
800.0	-0.329	2.318	2.575	2.788	2.997	3.062
850.0	-0.379	2.270	2.524	2.743	2.964	3.040
900.0	-0.429	2.226	2.474	2.699	2.933	3.018
950.0	-0.477	2.184	2.424	2.657	2.902	2.996
1000.0	-0.525	2.145	2.375	2.617	2.873	2.974
1050.0	-0.571	2.109	2.327	2.577	2.844	2.951
1100.0	-0.617	2.075	2.279	2.539	2.817	2.929
1150.0	-0.661	2.044	2.231	2.502	2.789	2.906
1200.0	-0.703	2.016	2.184	2.466	2.762	2.883
1250.0	-0.744	1.990	2.138	2.431	2.736	2.860
1300.0	-0.784	1.967	2.093	2.397	2.710	2.838
1350.0	-0.822	1.947	2.049	2.364	2.685	2.816
1400.0	-0.858	1.928	2.006	2.333	2.662	2.794