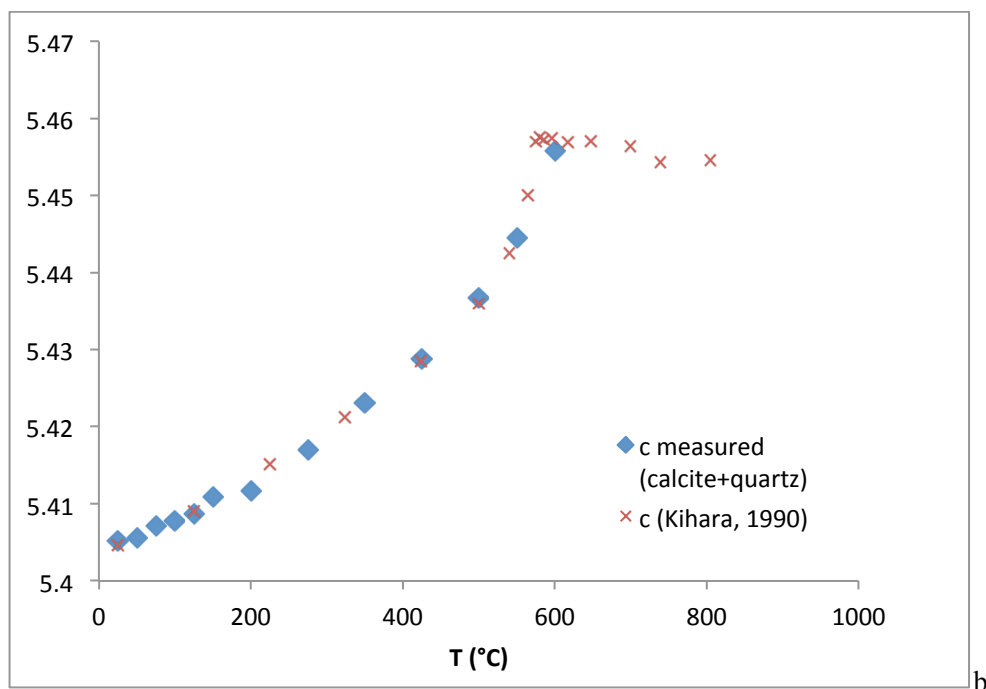
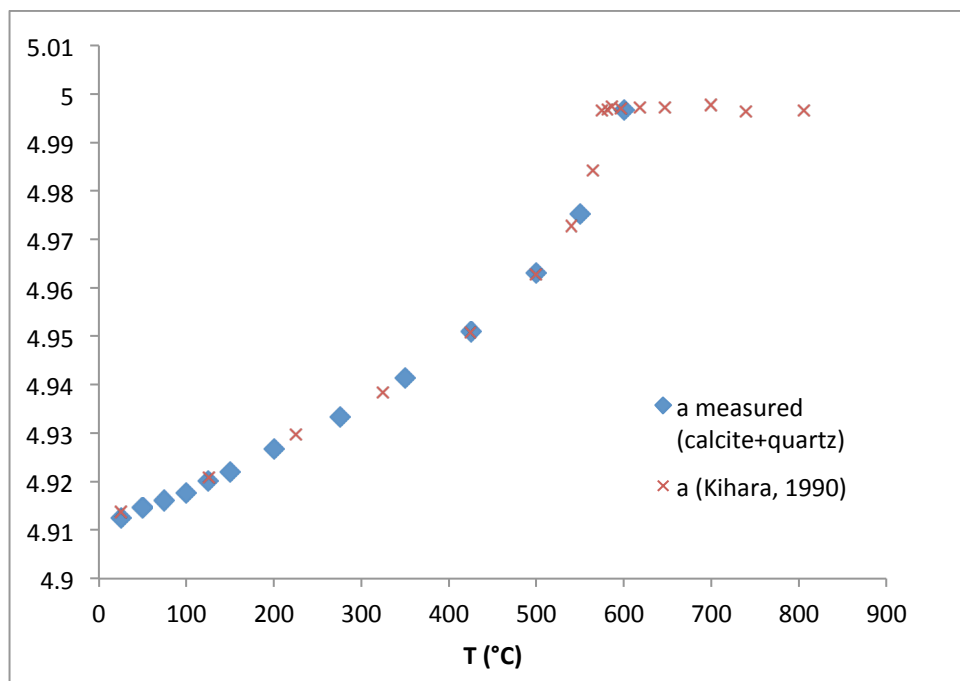


Deposit Items

Thermal expansion

In Fig. 1 the measured unit cell parameters of quartz added as internal standard are compared with reference ones (Kihara, 1990). The data are shown for the samples calcite and dolomite.



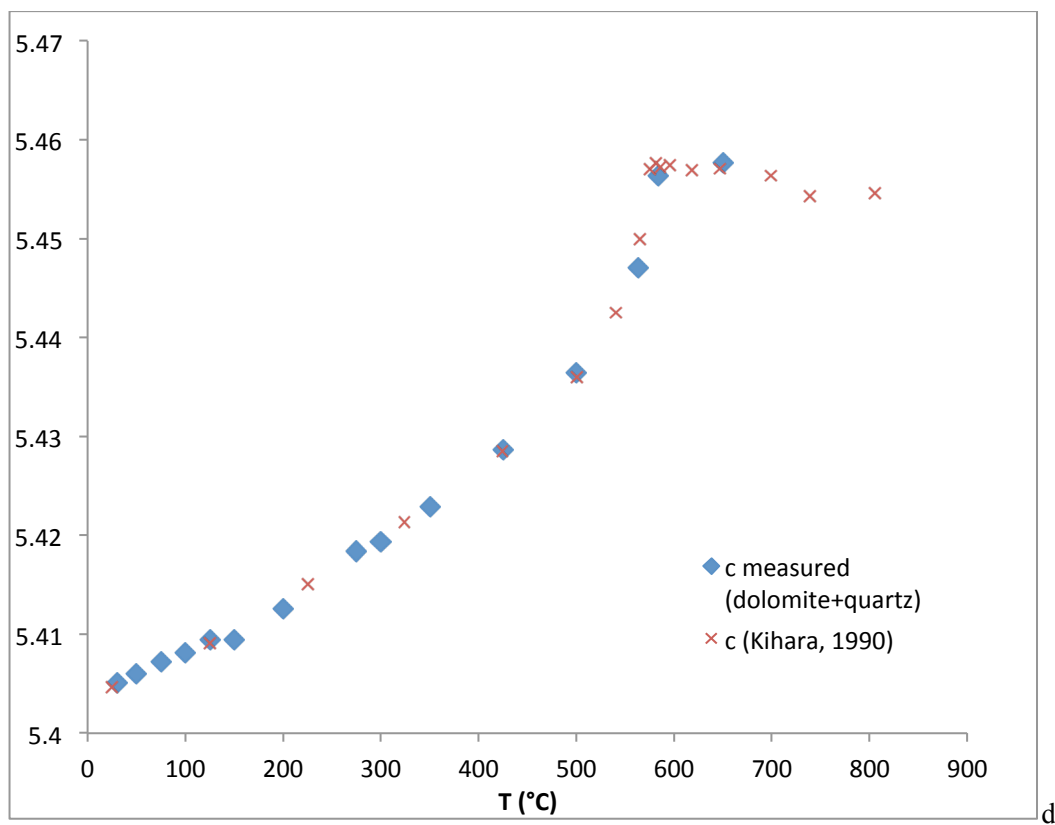
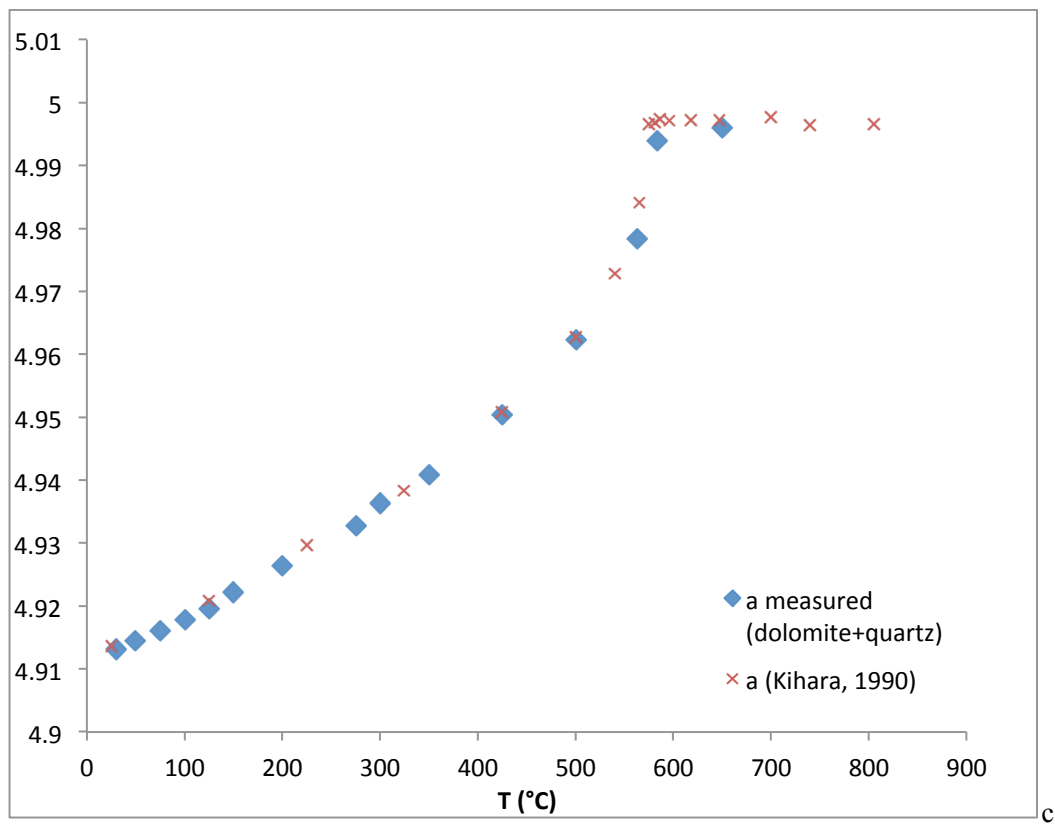


Fig. 1 – Measured lattice parameters of quartz at variable temperatures for the samples calcite+quartz and dolomite+quartz compared with literature data

The following tables report the measured unit cell parameters as function of temperature for the samples studied in the current work. The computed errors (GSAS) resulting from Rietveld fit are all in the range 0.0001-0.0002 for a, 0.0003-0.0005 for c and 0.01-0.02 for volume data respectively.

T (K)	a (Å)	c (Å)	V (Å ³)
298	4.9855	17.0428	366.83
323	4.9847	17.0533	366.95
348	4.9840	17.0643	367.08
373	4.9832	17.0765	367.23
398	4.9824	17.0878	367.35
423	4.9818	17.1008	367.55
473	4.9807	17.1228	367.86
548	4.9790	17.1645	368.50
623	4.9776	17.2029	369.11
698	4.9765	17.2457	369.87
773	4.9756	17.2892	370.67
823	4.9752	17.3198	371.26
873	4.9748	17.3499	371.84
299	4.9854	17.0442	366.85

Table 1 – Lattice parameters for the sample calcite

T (K)	a	c	Vol
298	4.9410	16.8465	356.18
323	4.9394	16.8675	356.40
373	4.9397	16.8846	356.80
423	4.9388	16.9070	357.14
473	4.9376	16.9295	357.45
523	4.9364	16.9563	357.84
573	4.9367	16.9852	358.49
623	4.9367	17.0153	359.12
673	4.9373	17.0478	359.90
723	4.9377	17.0805	360.65
773	4.9382	17.1070	361.27
823	4.9383	17.1370	361.93
873	4.9379	17.1686	362.54
923	4.9376	17.1986	363.13
973	4.9377	17.2298	363.80
1023	4.9379	17.2677	364.62
1073	4.9393	17.2987	365.49
1123	4.9447	17.3767	367.94

Table 2 – Lattice parameters for the sample (Ca_{0.91}Mg_{0.06}Fe_{0.03})CO₃

T (K)	a (Å)	c (Å)	V (Å ³)
303	4.8102	16.0262	321.12
323	4.8105	16.0313	321.27
348	4.8111	16.0412	321.55
373	4.8114	16.0492	321.75
398	4.8119	16.0578	321.98
423	4.8124	16.0668	322.23
473	4.8136	16.0871	322.80
548	4.8157	16.1145	323.63
573	4.8165	16.1246	323.95
623	4.8178	16.1455	324.53
698	4.8201	16.1771	325.48
773	4.8225	16.2100	326.47
836	4.8247	16.2381	327.33
856	4.8253	16.2469	327.60
923	4.8275	16.2777	328.51

Table 3 – Lattice parameters for the sample dolomite (Bazena)

T (K)	a (Å)	c (Å)	V (Å ³)
298	4.8189	16.0877	323.52
323	4.8193	16.0957	323.74
348	4.8197	16.1037	323.95
373	4.8202	16.1113	324.17
398	4.8208	16.1210	324.45
423	4.8211	16.1296	324.66
473	4.8224	16.1471	325.19
548	4.8244	16.1756	326.04
623	4.8266	16.2099	327.03
698	4.8286	16.2409	327.92
773	4.8307	16.2750	328.90
823	4.8322	16.2965	329.54
873	4.8338	16.3220	330.27

Table 4 – Lattice parameters for the sample Fe-dolomite (La Mure)

T (K)	a (Å)	c (Å)	V (Å ³)
298	4.6381	15.0386	280.17
323	4.6386	15.0464	280.37
348	4.6393	15.0555	280.62
373	4.6398	15.0634	280.83
398	4.6407	15.0725	281.12
423	4.6413	15.0801	281.32
473	4.6429	15.0994	281.88
523	4.6445	15.1171	282.40
573	4.6462	15.1348	282.94
623	4.6482	15.1549	283.56
673	4.6500	15.1755	284.16
723	4.6520	15.1950	284.77
773	4.6540	15.2151	285.39
823	4.6558	15.2357	286.01
873	4.6579	15.2574	286.67

Table 5 – Lattice parameters for the sample magnesite (Czeck)

T (K)	a	c	vol
298	4.6412	15.0556	280.86
323	4.6419	15.0632	281.09
348	4.6425	15.0713	281.32
373	4.6432	15.0801	281.56
398	4.6438	15.0882	281.79
423	4.6447	15.0949	282.01
473	4.6461	15.1135	282.54
523	4.6478	15.1327	283.11

Table 6 – Lattice parameters for the sample braunnerite (Fe-magnesite, Tyrol)

T (K)	a (Å)	c (Å)	V (Å ³)
298	4.6809	15.3140	290.58
323	4.6816	15.3203	290.78
348	4.6822	15.3285	291.02
373	4.6828	15.3347	291.21
398	4.6838	15.3410	291.46
423	4.6843	15.3512	291.71
473	4.6860	15.3671	292.23
523	4.6877	15.3810	292.70
573	4.6896	15.3999	293.29
623	4.6912	15.4182	293.85
673	4.6931	15.4355	294.42
299	4.6809	15.3127	290.56

Table 7 – Lattice parameters for the sample siderite (Puits de Villaret)

T (K)	a (Å)	c (Å)	V (Å ³)
298	4.6923	15.3836	293.32
323	4.6930	15.3907	293.54
348	4.6937	15.3971	293.76
373	4.6945	15.4045	294.00
398	4.6953	15.4128	294.26
423	4.6960	15.4204	294.49
473	4.6977	15.4357	294.99
523	4.6995	15.4499	295.50
573	4.7012	15.4658	296.02
623	4.7030	15.4828	296.56
673	4.7049	15.4995	297.12

Table 8 – Lattice parameters for the sample siderite (Ivigtut)

The following tables report the result of thermal expansion fit using the Pawley et al. (1996) – eq. 3 with two terms a_0 and a_1 (table 9) and a linear fit (table 10)

	V_0 (Å ³)	a_0 (K ⁻¹)*10 ⁵	a_1 (K ⁻²)*10 ⁴
Calcite	366.90(1)	6.25(14)	-9.1(3)
(Ca _{0.91} Mg _{0.06} Fe _{0.03})CO ₃	356.20(9)	7.4(4)	-10.2(11)
Dolomite (Bazena)	321.10(1)	6.73(9)	-7.2(2)
Fe-dolomite (La Mure)	323.50(2)	6.77(18)	-7.4(4)
Magnesite (Czeck)	280.20(1)	6.90(12)	-6.7(3)
Braunnerite (Tyrol)	280.90(1)	6.9(7)	-6.8(13)
Siderite (Puits de Villaret)	290.60(1)	6.4(2)	-6.3(6)
Siderite (Ivigtut)	293.30(1)	5.17(16)	-3.7(3)

Table 9 – Thermal expansion fit with eq. 3 (Pawley, 1996)

	V_0	a_0 *10 ⁵
calcite	366.60(8)	2.32(7)
(Ca _{0.91} Mg _{0.06} Fe _{0.03})CO ₃	355.70(14)	3.29(9)
Dolomite (Bazena)	320.80(6)	3.68(6)
Fe-dolomite (La Mure)	323.30(6)	3.60(6)
Magnesite (Czeck)	280.00(4)	4.00(5)
Braunnerite (Tyrol)	280.80(2)	3.51(6)
Siderite (Puits de Villaret)	290.50(3)	3.49(5)
Siderite (Ivigtut)	293.30(2)	3.43(3)

Table 10 – Thermal expansion fit with a linear equation

In the following tables the unit cell parameters at variable pressures are reported for the samples investigated

P (Gpa)	a	c	Vol
0.48	4.9523	16.844	357.77
0.69	4.9478	16.818	356.56
0.91	4.9469	16.787	355.77
1.21	4.9409	16.753	354.18
1.38	4.9383	16.732	353.36
1.59	4.935	16.699	352.2
1.9	4.9299	16.668	350.81
2.08	4.9264	16.645	349.84
2.28	4.9239	16.616	348.88
2.54	4.9178	16.583	347.33

Table 11 - $(\text{Ca}_{0.91}\text{Mg}_{0.06}\text{Fe}_{0.03})\text{CO}_3$

P (Gpa)	a	c	vol
0	4.8394	16.263	329.85
0.1	4.8375	16.249	329.31
2.04	4.8093	16.035	321.19
3.46	4.7945	15.911	316.75
5.51	4.7774	15.735	311.01
8.04	4.7483	15.540	303.43
9.22	4.7396	15.453	300.63
11.42	4.7146	15.295	294.42
12.56	4.7086	15.235	292.52
13.76	4.6964	15.154	289.46
15.26	4.6867	15.087	286.99
16.74	4.6710	15.010	283.62
16.74	4.6740	14.991	283.62
18.08	4.6635	14.934	281.27
19.63	4.6420	14.854	277.19
20.96	4.6350	14.764	274.68
22.53	4.6220	14.694	271.85
24.85	4.6050	14.574	267.65

Table 12 – $(\text{Ca}_{0.55}\text{Mg}_{0.45})\text{CO}_3$ disordered dolomite

P (Gpa)	a (Å)	c (Å)	V (Å ³)
0	4.8078	16.008	320.44
3.44	4.7805	15.695	310.62
5.54	4.7589	15.501	304.01
7.31	4.7468	15.355	299.62
9.5	4.7291	15.202	294.43
11.91	4.7133	15.037	289.29
14.41	4.7012	14.866	284.53

Table 13 - Dolomite

P (Gpa)	a (Å)	c (Å)	V (Å ³)
0	4.8177	16.091	323.44
0.18	4.8162	16.074	322.9
0.99	4.8072	15.981	319.84
5.11	4.771	15.601	307.55
9.43	4.7414	15.272	297.33
14.19	4.699	14.98	286.45

Table 14 – Fe-dolomite

P	a	c	vol
average			
0	4.635	15.013	279.3
3.49	4.6025	14.78	271.2
5.11	4.5875	14.678	267.5
7.21	4.5656	14.532	262.3
9.17	4.5532	14.442	259.3
10.95	4.5421	14.359	256.5
12.54	4.5338	14.283	254.3
13.95	4.5258	14.242	252.6
15.31	4.5166	14.178	250.5
16.92	4.5079	14.113	248.4
18.83	4.496	14.043	245.8
21.08	4.4815	13.935	242.37
23.38	4.4697	13.864	239.2
25.27	4.4626	13.776	237.6
27.93	4.4505	13.695	234.91
30.08	4.4396	13.626	232.59
32.48	4.4276	13.544	229.94
34.31	4.4147	13.485	227.6
36.54	4.3988	13.41	224.7
39.74	4.3947	13.345	223.2

Table 15 – Magnesite

P (Gpa)	a	c	vol
0.00	4.6399	15.0612	280.81
0.16	4.6423	15.067	281.21
2.02	4.6189	14.918	275.62
4.91	4.5994	14.794	271.03
6.55	4.587	14.647	266.89
8.66	4.5731	14.533	263.21
14.13	4.5325	14.248	253.49
16.71	4.5202	14.14	250.20
19.65	4.5047	14.024	246.45
23.40	4.4863	13.878	241.90
27.24	4.4694	13.734	237.59
31.11	4.4554	13.588	233.59
33.06	4.4444	13.526	231.38

36.05	4.4318	13.435	228.52
39.34	4.4228	13.335	225.90
42.35	4.4118	13.252	223.38
45.75	4.3914	13.129	219.26
48.75	4.3772	13.018	216.01
51.77	4.3639	12.942	213.44
54.86	4.3545	12.876	211.44
57.62	4.3483	12.796	209.53
60.61	4.3382	12.727	207.43
62.25	4.336	12.663	206.18
63.97	4.331	12.628	205.14
65.95	4.3241	12.633	204.56
68.88	4.3147	12.575	202.74
71.49	4.3059	12.53	201.19
74.07	4.3002	12.463	199.59
75.87	4.2952	12.447	198.87
77.71	4.2898	12.416	197.87
80.77	4.2809	12.343	195.89
84.39	4.2767	12.297	194.78
88.08	4.2653	12.213	192.42
91.00	4.262	12.15	191.13
94.23	4.255	12.13	190.19
97.00	4.251	12.077	189.00
99.84	4.261	12.09	190.10
100.93	4.2386	12.049	187.47

Table 16 – Fe-magnesite (braunnerite)

P (Gpa)	a	c	vol
0	4.6738	15.271	288.89
4.53	4.64	14.954	278.82
6.23	4.6279	14.836	275.18
7.82	4.6108	14.724	271.09
10.58	4.5943	14.5726	266.38
14.39	4.5772	14.388	261.05
17.71	4.564	14.237	256.83
20.56	4.5557	14.107	253.56
22.88	4.5447	14.011	250.62
24.51	4.5365	13.938	248.41
27.08	4.5256	13.828	245.27
29.85	4.5115	13.712	241.7
32.74	4.503	13.625	239.26
36.53	4.493	13.501	236.03
38.73	4.4858	13.417	233.81
40.45	4.4829	13.375	232.78
41.91	4.4798	13.318	231.47
43.25	4.4723	13.266	229.79

Table 17 – siderite Puits de Villaret

P (Gpa)	a	c	vol
0	4.6899	15.351	292.40
15.1	4.5931	14.420	263.45
19.2	4.5737	14.206	257.35
22.85	4.5594	14.051	252.96
27	4.5404	13.896	248.07
31	4.5286	13.738	243.99
35.2	4.5165	13.590	240.06
39.3	4.5089	13.458	236.95
43.4	4.4977	13.318	233.32
46.5	4.3869	12.838	213.95
49.5	4.3775	12.750	211.59
52.3	4.3723	12.685	210.01
46	4.3907	12.837	214.31
43.5	4.5048	13.282	233.41

Table 18 – Siderite Foppolo

P (Gpa)	a	c	vol
0.18	4.6900	15.380	292.96
0.99	4.6836	15.310	290.83
5.11	4.6550	15.023	281.91
9.43	4.6284	14.740	273.45
14.19	4.6047	14.498	266.22
19.53	4.5787	14.198	257.76
24.47	4.5636	13.949	251.57
29.65	4.5494	13.723	245.97
34.34	4.5378	13.531	241.29
39.88	4.5227	13.298	235.56

Table 19 – Siderite Ivigtut

Selected F-f plot for the samples $(\text{Ca}_{0.91}\text{Mg}_{0.06}\text{Fe}_{0.03})\text{CO}_3$ (Fig. 2), disordered dolomite (Fig. 3) and Fe-magnesite (braunnerie), Fig. 4.

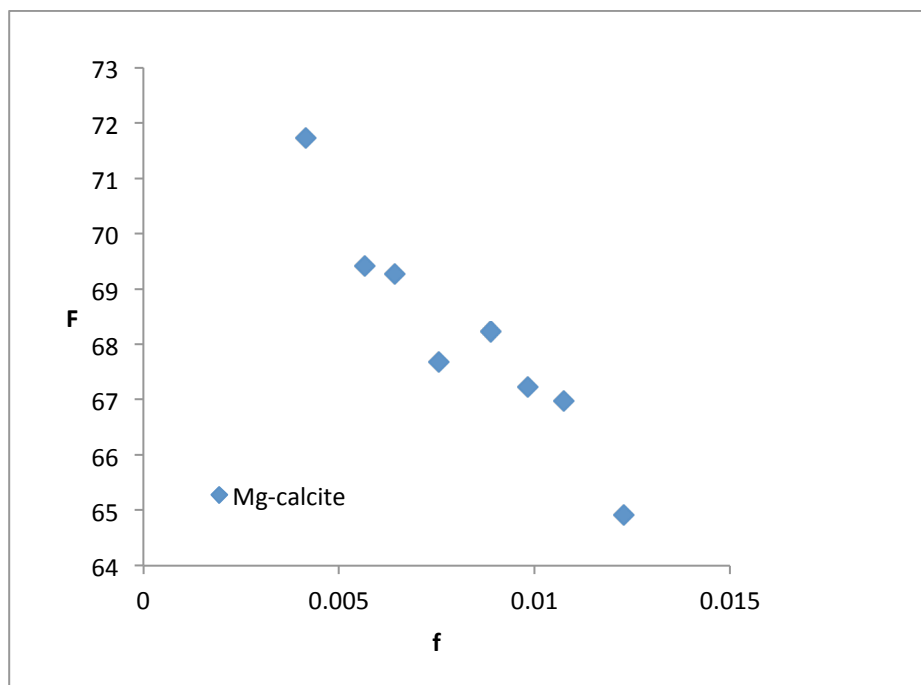


Fig. 2 – F-f plot for the sample $(\text{Ca}_{0.91}\text{Mg}_{0.06}\text{Fe}_{0.03})\text{CO}_3$. A 3rd order BM should be used with $K' < 4$

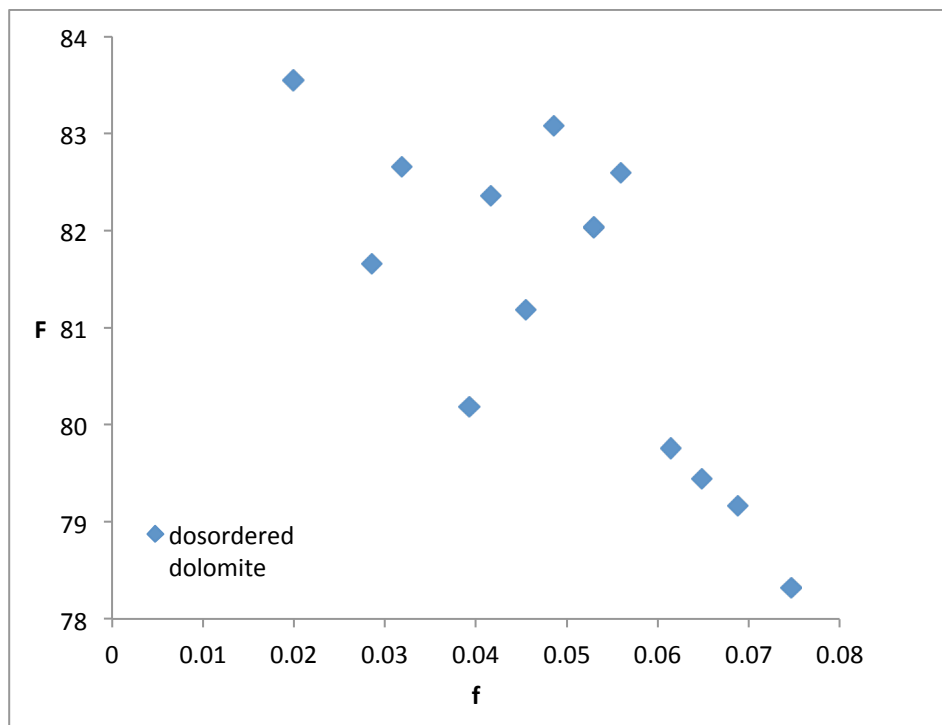


Fig. 3 – F-f plot for the sample disordered dolomite. A 3rd order BM should be used with $K' < 4$

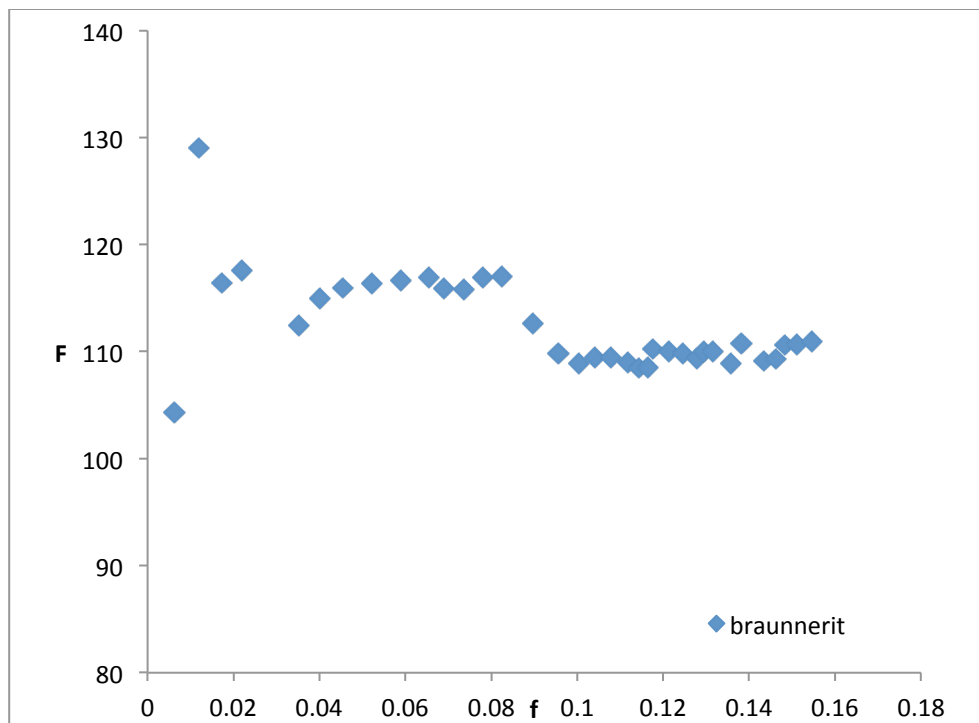


Fig. 3 – F-f plot for the sample Fe-magnesite (braunnerite). The high to low spin transition of Fe atoms is visible, for values $f=0.1$ (corresponding to pressure interval 43-48 GPa). For the 0-40 GPa interval a BM with $K'=4$ is correct.

In the following tables (table 20 and table 21) the lattice parameters for the sample dolomite (table 20) and Fe-dolomite (table 21) are reported at variable pressures and temperatures. The computed volume from the equation of states reported in the current work is reported, and, for comparison, also the computed volume for pure calcite and magnesite

T (°C)	T (K)	P (GPa)	a	c	Vol	calculated	difference	V calc magnesite	Vol calc calcite
750	1023	3.83	4.783	15.8436	313.85	315.829	-1.9787	278.083	354.021
800	1073	3.83	4.785	15.8628	314.57	316.422	-1.8534	278.704	354.419
850	1123	3.85	4.787	15.9	315.55	316.964	-1.4149	279.292	354.741
950	1223	1.64	4.811	16.2402	325.45	326.472	-1.0219	286.455	367.821
950	1223	1.88	4.81	16.2417	325.39	325.526	-0.1338	285.791	366.399
950	1223	2.37	4.805	16.1785	323.43	323.635	-0.2042	284.46	363.576
1000	1273	2.56	4.802	16.1986	323.41	323.64	-0.2338	284.676	363.107
1000	1273	2.643	4.801	16.1954	323.24	323.324	-0.0806	284.453	362.637
1050	1323	2.88	4.795	16.2237	323.02	323.154	-0.1297	284.552	361.904
1075	1348	3.1	4.795	16.2233	322.97	322.686	0.2859	284.333	360.968
1100	1373	3.22	4.792	16.2317	322.72	322.598	0.1228	284.384	360.594
1150	1423	3.4	4.792	16.2596	323.33	322.653	0.6784	284.654	360.18
1200	1473	3.611	4.789	16.2827	323.42	322.595	0.8299	284.849	359.59
1200	1473	3.91	4.792	16.2113	322.38	321.468	0.9077	284.049	357.929
1250	1523	4.08	4.789	16.1657	321.11	321.564	-0.4536	284.36	357.558
1300	1573	4.22	4.787	16.2048	321.53	321.777	-0.2433	284.761	357.35
1350	1623	4.32	4.785	16.2307	321.88	322.147	-0.2688	285.28	357.362
1400	1673	4.41	4.78	16.216	320.81	322.563	-1.7482	285.837	357.43
1450	1723	4.55	4.782	16.2318	321.42	322.791	-1.3698	286.268	357.209
1450	1723	4.59	4.781	16.2065	320.77	322.595	-1.8272	286.158	356.981

Table 20 – Volume of dolomite at variable pressures and temperatures and computed volume with the reported equations of state

T (°C)	T (K)	P (GPa)	a	c	Vol	V calc	diff	V calc calcite	V calc magnesite
25	298	2.14	4.7993	15.9379	317.92	316.411	1.5087627	356.787	274.517
150	423	2.22	4.8005	15.9549	318.42	317.162	1.2560411	356.792	275.427
300	573	2.36	4.8022	15.9831	319.21	318.064	1.1428005	356.799	276.541
450	723	2.52	4.8052	16.0115	320.17	319.049	1.1246509	356.91	277.738
627	900	2.72	4.8088	16.045	321.32	320.356	0.9684575	357.221	279.288
627	900	2.79	4.8088	16.0449	321.32	320.11	1.2124549	356.873	279.116
627	900	2.78	4.8087	16.0474	321.36	320.145	1.2141552	356.923	279.141
627	900	2.78	4.8089	16.049	321.42	320.145	1.2729309	356.923	279.141
677	950	1.23	4.8262	16.2455	327.70	326.497	1.201418	365.596	283.723
777	1050	1.6	4.8223	16.2654	327.57	326.461	1.1087801	364.642	284.086
826	1099	1.85	4.8169	16.2704	326.94	326.188	0.749037	363.796	284.094
900	1173	2.64	4.8043	16.2132	324.09	324.203	-0.1174936	360.236	283.033
950	1223	2.78	4.8032	16.2335	324.34	324.383	-0.0402922	360.021	283.368
1000	1273	2.38	4.8095	16.271	325.95	326.681	-0.7356911	362.866	285.164
1050	1323	2.3	4.8124	16.2953	326.83	327.776	-0.9501282	363.972	286.133
1130	1403	2.43	4.8086	16.3682	327.77	328.524	-0.7542583	364.263	287.006
1170	1443	2.55	4.8072	16.3283	326.78	328.681	-1.9006115	364.084	287.301
1170	1443	2.59	4.806	16.288	325.81	328.516	-2.7048631	363.842	287.189
1200	1473	2.63	4.8008	16.2959	325.26	328.844	-3.5798415	364.01	287.076
1240	1513	2.69	4.8031	16.331	326.28	329.26	-2.9828442	364.197	288.031
1240	1513	2.74	4.8032	16.2893	325.46	329.051	-3.5934172	363.891	287.889

Table 20 – Volume of Fe-dolomite at variable pressures and temperatures and computed volume with the reported equations of state