

Supplementary information

Table S1 – Lattice parameters and atomic coordinates of Fe-dolomite-IIIb obtained from crystal structure determination and refinement using the experimental dataset collected at 38.19 GPa.

Formula sum	Ca(Mg _{0.6} Fe _{0.4})(CO ₃) ₂
Crystal system	trigonal
Space group	<i>R</i> 3 (no. 146)
Unit cell dimensions	<i>a</i> = 11.970(3) Å <i>c</i> = 13.664(5) Å
Cell volume	1695.5(9) Å ³
Z	21

Atomic coordinates and isotropic displacement parameters (in Å²)

Atom	Wyck.	Occ.	x	y	z	U
Mg1	3 <i>a</i>	0.608	2/3	1/3	0.13121	0.0079
Fe1	3 <i>a</i>	0.392	2/3	1/3	0.13121	0.0079
Mg2	9 <i>b</i>	0.637	0.39166	0.46493	0.14985	0.0092
Fe2	9 <i>b</i>	0.363	0.39166	0.46493	0.14985	0.0092
Mg3	9 <i>b</i>	0.579	0.60219	0.52688	0.45639	0.0146
Fe3	9 <i>b</i>	0.421	0.60219	0.52688	0.45639	0.0146
Ca1	9 <i>b</i>		0.58980	0.73611	0.27277	0.0078
Ca2	9 <i>b</i>		0.41042	0.26353	0.32805	0.0138
Ca3	3 <i>a</i>		1.00000	1.00000	0.33006	0.0142
O1	9 <i>b</i>		0.50568	0.43127	0.22710	0.0077
O2	9 <i>b</i>		0.49282	0.56761	0.36371	0.0118
O3	9 <i>b</i>		0.51061	0.22163	0.20705	0.0074
O4	9 <i>b</i>		0.37564	0.38738	0.43242	0.0036
O5	9 <i>b</i>		0.64012	0.62339	0.17253	0.0215
O6	9 <i>b</i>		0.60931	0.39827	0.38192	0.0110
O7	9 <i>b</i>		0.54861	0.37935	0.05780	0.0115
O8	9 <i>b</i>		0.89883	0.78629	0.42384	0.0145
O9	9 <i>b</i>		0.71499	0.66145	0.34178	0.0228
O10	9 <i>b</i>		0.78055	0.86655	0.36832	0.0115
O11	9 <i>b</i>		0.77044	0.87989	0.16909	0.0186
O12	9 <i>b</i>		0.38471	0.59796	0.22406	0.0086
O13	9 <i>b</i>		0.27828	0.32857	0.25834	0.0003
O14	9 <i>b</i>		0.54729	0.40505	0.56884	0.0138
C1	3 <i>a</i>		1/3	2/3	0.22029	0.0109
C2	9 <i>b</i>		0.62134	0.51788	0.20450	0.0051
C3	9 <i>b</i>		0.18761	0.22543	0.22275	0.0001
C4	9 <i>b</i>		0.79183	0.76797	0.38519	0.0215
C5	3 <i>a</i>		0	0	0.05337	0.0114
C6	9 <i>b</i>		0.04917	0.82231	0.72375	0.0122

Figure S1 – Observed (F_{obs}) and calculated (F_{calc}) structure factors after crystal structure refinement of the dolomite-IIIb polymorph. All the parameters (atomic coordinates, isotropic displacement factors) have been refined without constraints. The refinements converged to an R_{Bragg} value of 7.09 % and a weighted R_{Bragg} of 5.81 % (R_{Bragg} defined according to the Jana2006 software, Petricek et al. 2016). The number of refined parameters is 100 and the number of unique diffraction is 1617 (746 with $I/\sigma(I) > 3$).

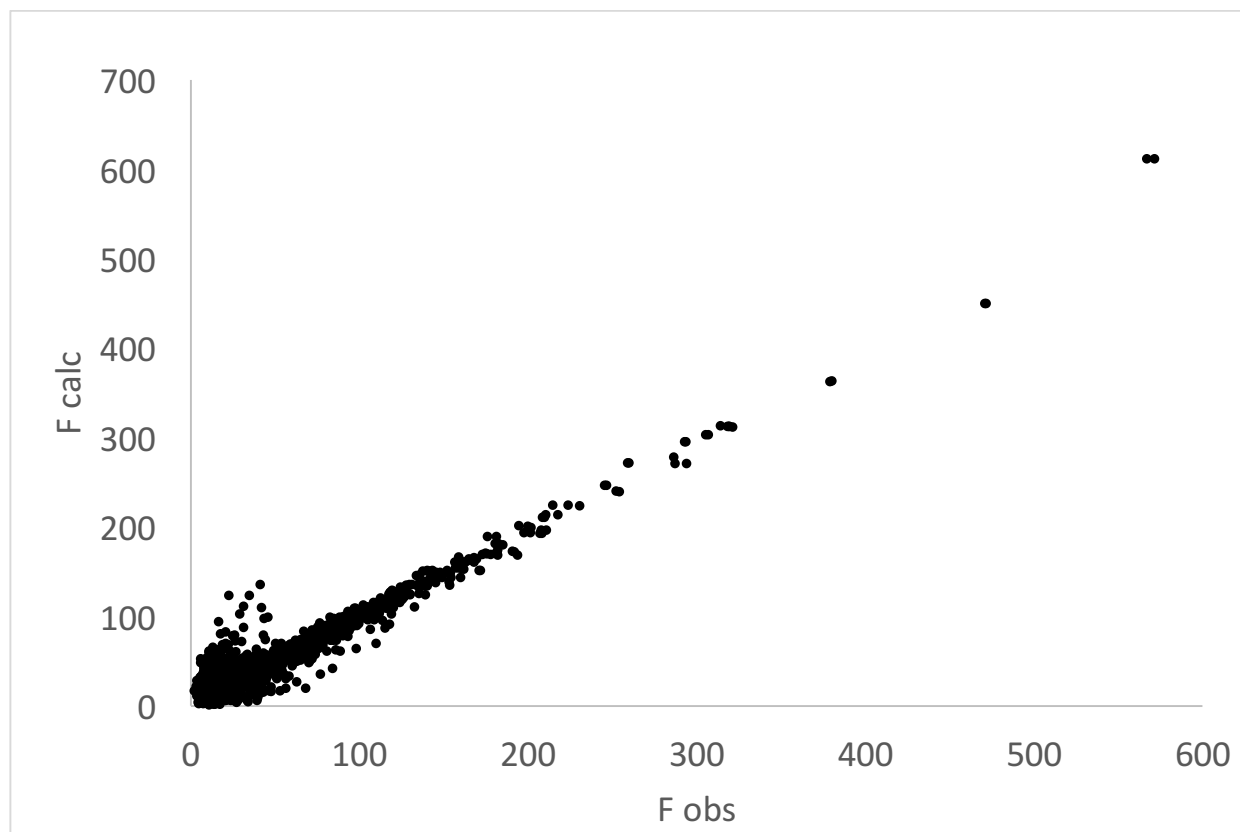


Table S2 – Lattice parameters and atomic coordinates of Fe-dolomite-IV obtained from crystal structure determination and refinement using the experimental dataset collected at 115.18 GPa.

Formula sum	(Ca _{0.5} Mg _{0.3} Fe _{0.2})CO ₃
Crystal system	orthorhombic
Space group	<i>P</i> n m a (no. 62)
Unit cell dimensions	<i>a</i> = 10.091(3) Å <i>b</i> = 8.090(7) Å <i>c</i> = 4.533(3) Å
Cell volume	370.06(40) Å ³
Z	12

Atomic coordinates and isotropic displacement parameters (in Å²)

Atom	Wyck.	Occ.	x	y	z	U
Ca1	8 <i>d</i>	0.5	0.38668	0.42108	-0.12920	0.0344
Mg1	8 <i>d</i>	0.3	0.38668	0.42108	-0.12920	0.0344
Fe1	8 <i>d</i>	0.2	0.38668	0.42108	-0.12920	0.0344
Ca2	4 <i>c</i>	0.5	0.28699	3/4	-0.11790	0.0198
Mg2	4 <i>c</i>	0.3	0.28699	3/4	-0.11790	0.0198
Fe2	4 <i>c</i>	0.2	0.28699	3/4	-0.11790	0.0198
O1	4 <i>c</i>		0.89928	1/4	-0.09392	0.0224
O2	8 <i>d</i>		0.94877	0.62123	-0.09529	0.0158
O3	4 <i>c</i>		0.60528	3/4	-0.13718	0.0296
O4	8 <i>d</i>		0.57311	0.39694	-0.11078	0.0159
O5	4 <i>c</i>		0.21186	1/4	-0.09242	0.0064
O6	8 <i>d</i>		0.21655	0.49650	-0.01843	0.0432
C1	8 <i>d</i>		0.12914	0.39689	-0.10755	0.0163
C2	4 <i>c</i>		0.03668	3/4	-0.14980	0.0155

Figure S2 – Observed (F_{obs}) and calculated (F_{calc}) structure factors after crystal structure refinements. All the parameters (atomic coordinates, isotropic displacement factors) have been refined without constraints. The refinements converged to an R_{Bragg} value of 9.28 % and a weighted R_{Bragg} of 5.95 % (R_{Bragg} defined according to the Jana2006 software, Petricek et al. 2016). The number of refined parameters is 36 and the number of unique diffraction is 351 (105 with $I/\sigma(I) > 3$)

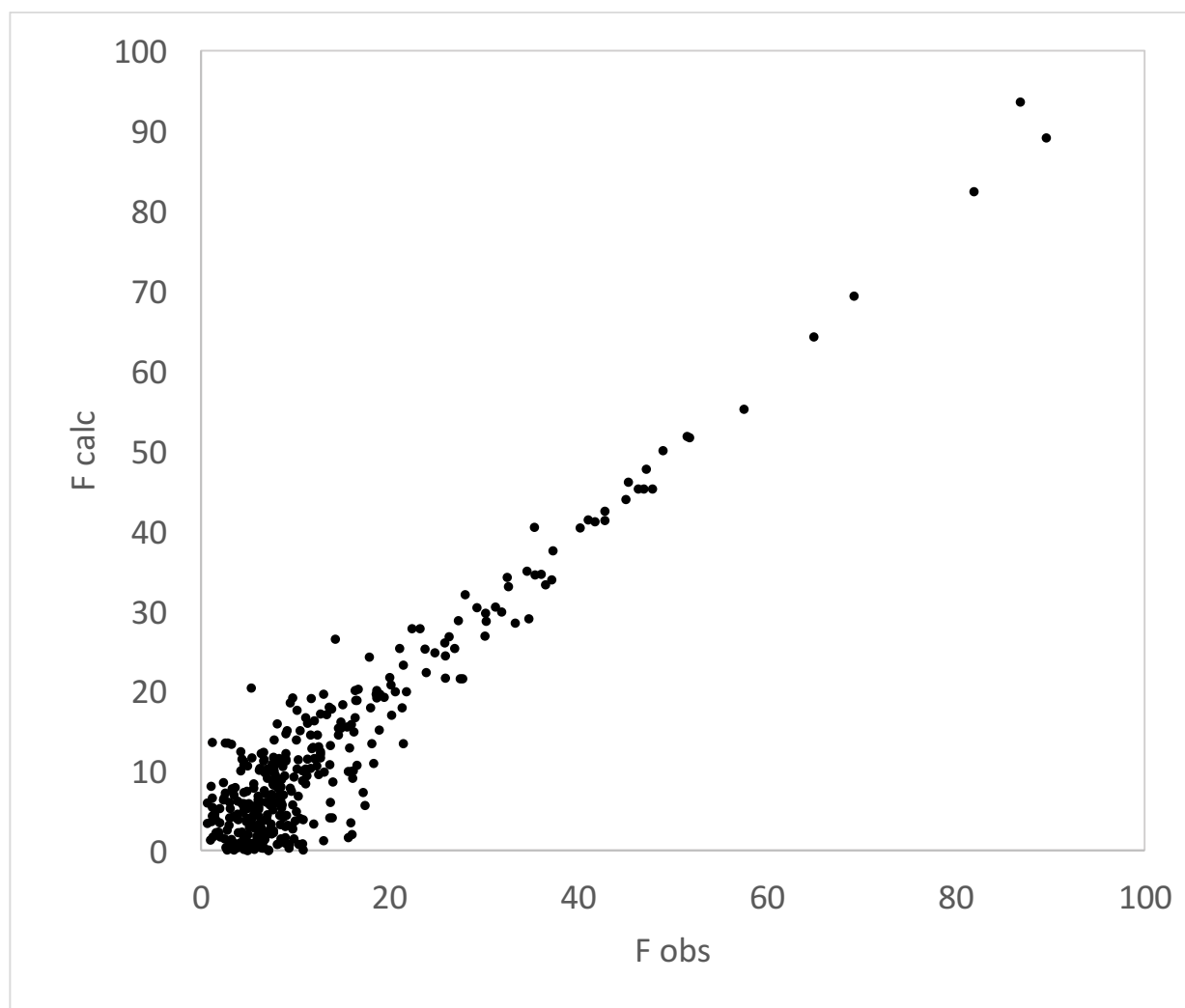


Table S3 – Lattice parameters, normalized volume and density of the Fe-dolomite polymorphs. The errors are reported in a following table.

Structure	P (GPa)	vol V/Z	ρ (g/cm ³)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å ³)
Fe-dolomite	0	107.68	3.039	4.81649		16.079				323.04
Fe-dolomite	0.34	107.23	3.052	4.8126		16.038				321.69
Fe-dolomite	0.78	106.79	3.065	4.808		16.003				320.38
Fe-dolomite	1.2	106.44	3.075	4.8058		15.965				319.32
Fe-dolomite	3.65	103.99	3.147	4.7846		15.7356				311.96
Fe-dolomite	6.53	101.4	3.228	4.7619		15.49				304.19
Fe-dolomite	9.36	99.14	3.301	4.7419		15.274				297.43
Fe-dolomite	12.02	96.81	3.381	4.7212		15.0461				290.44
Fe-dolomite	13.78	95.47	3.428	4.715		14.877				286.42
Fe-dol-II	15.58	93.95	3.484	4.7293	5.6217	7.282	103.84	89.74	91.62	187.9
Fe-dol-II	16.95	93.06	3.517	4.7333	5.599	7.236	103.77	89.62	92.23	186.12
Fe-dol-II	18.6	91.91	3.561	4.7321	5.5723	7.179	103.57	89.58	92.698	183.82
Fe-dol-II	20.13	90.9	3.601	4.7321	5.5469	7.128	103.36	89.52	93.06	181.79
Fe-dol-II	21.72	90.14	3.631	4.7339	5.526	7.091	103.2	89.41	93.38	180.28
Fe-dol-II	23.44	89.3	3.665	4.7344	5.5042	7.05	103.05	89.32	93.7	178.6
Fe-dol-II	25.07	88.31	3.706	4.7271	5.4815	7.006	102.81	89.42	93.84	176.61
Fe-dol-II	27.93	86.7	3.775	4.7076	5.4461	6.946	102.52	89.59	94.06	173.4
Fe-dol-II	29.32	86.04	3.804	4.7035	5.4273	6.921	102.36	89.53	94.28	172.08
Fe-dol-II	30.08	85.99	3.806	4.7173	5.4144	6.905	102.02	89.31	94.4	171.97
Fe-dol-II	31.33	85.42	3.831	4.7187	5.4044	6.867	101.89	89.28	94.53	170.84
Fe-dol-II	32.89	84.8	3.859	4.7197	5.387	6.836	101.71	89.27	94.78	169.6
Fe-dol-II	33.98	84.38	3.879	4.7191	5.3761	6.816	101.61	89.23	94.95	168.76
Fe-dol-II	35.66	83.85	3.903	4.73	5.345	6.784	101.03	89.27	94.98	167.7
Fe-dol-IIIb	36.81	81.49	4.016	12.01		13.7				1711.34
Fe-dol-IIIb	38.19	80.74	4.054	11.97		13.664				1695.5
Fe-dol-IIIb	39.42	80.33	4.074	11.9561		13.626				1686.86
Fe-dol-IIIb	41.85	79.63	4.11	11.9356		13.554				1672.19
Fe-dol-IIIb	43.48	79.13	4.136	11.9168		13.511				1661.64
Fe-dol-IIIb	46.28	78.17	4.187	11.8758		13.44				1641.56
Fe-dol-IIIb	51.27	76.8	4.261	11.824		13.321				1612.86
Fe-dol-IIIb	53.45	76.27	4.291	11.82		13.237				1601.6
Fe-dol-IIIb	55.53	75.68	4.325	11.809		13.159				1589.2
Fe-dol-IIIb	57.55	75.18	4.354	11.782		13.132				1578.7
Fe-dol-IIIb	59.45	74.69	4.382	11.762		13.091				1568.43
Fe-dol-IIIb	61.45	74.21	4.41	11.742		13.051				1558.33
Fe-dol-IIIb	62.72	73.76	4.437	11.692		13.084				1548.99
Fe-dol-IIIb	64.72	73.3	4.465	11.681		13.026				1539.22
Fe-dol-IIIb	67.34	72.82	4.494	11.685		12.933				1529.28
Fe-dol-IIIb	68.19	72.53	4.512	11.648		12.963				1523.14
Fe-dol-IIIb	69.3	72.26	4.529	11.657		12.895				1517.49
Fe-dol-IIIb	71.23	71.8	4.558	11.639		12.852				1507.76
Fe-dol-IIIb	73.45	71.26	4.593	11.626		12.785				1496.55
Fe-dol-IIIb	75.83	70.84	4.62	11.617		12.728				1487.57
Fe-dol-IIIb	77.87	70.32	4.654	11.604		12.664				1476.78
Fe-dol-IIIb	80.04	69.88	4.684	11.588		12.619				1467.48
Fe-dol-IIIb	82.84	69.44	4.713	11.56		12.6				1458.2
Fe-dol-IIIb	85.28	68.99	4.744	11.54		12.562				1448.78
Fe-dol-IIIb	87.92	68.57	4.773	11.527		12.514				1439.99
Fe-dol-IIIb	90.27	68.14	4.803	11.53		12.429				1430.95
Fe-dol-IIIb	93.22	67.63	4.839	11.51		12.379				1420.26
Fe-dol-IIIb	96.2	67.04	4.882	11.512		12.267				1407.9
Fe-dol-IIIb	97.85	66.72	4.905	11.508		12.217				1401.18
Fe-dol-IIIb	99.99	66.59	4.915	11.472		12.269				1398.36

Fe-dol-IIIb	102.49	66.2	4.944	11.464		12.215				1390.26
Fe-dol-IIIb	104.49	65.95	4.962	11.457		12.184				1385.04
Fe-dol-IIIb	107.32	65.48	4.998	11.449		12.113				1375.05
Fe-dol-IIIb	109.36	65.24	5.016	11.444		12.08				1370.1
Fe-dol-IIIb	111.2	65	5.035	11.447		12.029				1365.03
Fe-dol-IV	115.89	63.17	5.181	4.577	8.09	10.236				379.02
Fe-dol-IV	115.18	61.68	5.306	4.533	8.09	10.091				370.06
Fe-dol-IV	114.58	62.19	5.263	4.556	8.089	10.125				373.14
Fe-dol-IV	114.12	62.26	5.256	4.553	8.1	10.13				373.59
Fe-dol-IV	113.39	62.11	5.27	4.543	8.103	10.123				372.65
Fe-dol-IV	113.95	61.97	5.281	4.546	8.095	10.104				371.83
Fe-dol-IV	112.92	62.18	5.263	4.547	8.141	10.079				373.1
Fe-dol-IV	111.71	63.41	5.162	4.602	8.12	10.181				380.45
Fe-dol-IV	109.24	62.85	5.207	4.555	8.157	10.15				377.12
Fe-dol-IV	107.91	62.88	5.205	4.557	8.155	10.152				377.27
Fe-dol-IV	106.02	64.19	5.099	4.613	8.194	10.189				385.13
Fe-dol-IV	104	64.53	5.072	4.563	8.291	10.234				387.17
Fe-dol-IV	102.45	64.54	5.071	4.57	8.24	10.283				387.22
Fe-dol-IV	98.93	64.66	5.062	4.578	8.28	10.235				387.97
Fe-dol-IV	94.92	65.79	4.975	4.611	8.32	10.289				394.72
Fe-dol-IV	90.31	67.12	4.876	4.64	8.41	10.32				402.71
Fe-dol-IV	85.18	67.62	4.84	4.647	8.446	10.337				405.71
Fe-dol-IV	77.85	68.57	4.773	4.702	8.397	10.421				411.45
Fe-dol-IV	68.55	68.32	4.791	4.661	8.47	10.383				409.91

Structure	P (GPa)	$\sigma(a)$	$\sigma(b)$	$\sigma(c)$	$\sigma(\alpha)$	$\sigma(\beta)$	$\sigma(\gamma)$	$\sigma(V)$
Fe-dolomite	0	0.0003		0.001				0.1
Fe-dolomite	0.34	0.0003		0.001				0.1
Fe-dolomite	0.78	0.0003		0.001				0.1
Fe-dolomite	1.2	0.0003		0.001				0.1
Fe-dolomite	3.65	0.0003		0.001				0.1
Fe-dolomite	6.53	0.0003		0.001				0.1
Fe-dolomite	9.36	0.0003		0.001				0.1
Fe-dolomite	12.02	0.0003		0.001				0.1
Fe-dolomite	13.78	0.0003		0.001				0.1
Fe-dol-II	15.58	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	16.95	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	18.6	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	20.13	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	21.72	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	23.44	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	25.07	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	27.93	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	29.32	0.0019	0.0015	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	30.08	0.0019	0.0019	0.003	0.03	0.04	0.03	0.13
Fe-dol-II	31.33	0.0018	0.0018	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	32.89	0.0018	0.0018	0.003	0.03	0.03	0.03	0.12
Fe-dol-II	33.98	0.0017	0.0018	0.003	0.03	0.03	0.03	0.11
Fe-dol-II	35.66	0.003	0.003	0.005	0.06	0.06	0.04	0.12
Fe-dol-IIIb	36.81	0.003		0.005				0.5
Fe-dol-IIIb	38.19	0.003		0.005				0.5
Fe-dol-IIIb	39.42	0.003		0.005				0.5
Fe-dol-IIIb	41.85	0.003		0.005				0.5
Fe-dol-IIIb	43.48	0.003		0.005				0.5

Fe-dol-IIIb	46.28	0.003		0.005				0.5
Fe-dol-IIIb	51.27	0.003		0.005				0.5
Fe-dol-IIIb	53.45	0.003		0.005				0.5
Fe-dol-IIIb	55.53	0.003		0.005				0.5
Fe-dol-IIIb	57.55	0.003		0.005				0.5
Fe-dol-IIIb	59.45	0.003		0.005				0.5
Fe-dol-IIIb	61.45	0.003		0.005				0.5
Fe-dol-IIIb	62.72	0.003		0.005				0.5
Fe-dol-IIIb	64.72	0.003		0.005				0.9
Fe-dol-IIIb	67.34	0.003		0.007				0.5
Fe-dol-IIIb	68.19	0.003		0.006				0.7
Fe-dol-IIIb	69.3	0.003		0.007				0.6
Fe-dol-IIIb	71.23	0.004		0.008				0.8
Fe-dol-IIIb	73.45	0.004		0.008				0.8
Fe-dol-IIIb	75.83	0.004		0.009				0.8
Fe-dol-IIIb	77.87	0.004		0.008				0.8
Fe-dol-IIIb	80.04	0.004		0.01				0.8
Fe-dol-IIIb	82.84	0.004		0.008				0.8
Fe-dol-IIIb	85.28	0.004		0.008				0.8
Fe-dol-IIIb	87.92	0.005		0.01				0.8
Fe-dol-IIIb	90.27	0.005		0.01				0.8
Fe-dol-IIIb	93.22	0.006		0.012				0.7
Fe-dol-IIIb	96.2	0.006		0.012				0.7
Fe-dol-IIIb	97.85	0.006		0.012				0.7
Fe-dol-IIIb	99.99	0.006		0.013				0.5
Fe-dol-IIIb	102.49	0.006		0.013				0.5
Fe-dol-IIIb	104.49	0.006		0.013				0.5
Fe-dol-IIIb	107.32	0.006		0.012				0.4
Fe-dol-IIIb	109.36	0.006		0.012				0.5
Fe-dol-IIIb	111.2	0.005		0.011				0.4
Fe-dol-IV	115.89	0.012	0.03	0.01				1
Fe-dol-IV	115.18	0.003	0.007	0.003				0.5
Fe-dol-IV	114.58	0.003	0.008	0.004				0.6
Fe-dol-IV	114.12	0.003	0.007	0.003				0.5
Fe-dol-IV	113.39	0.002	0.006	0.002				0.5
Fe-dol-IV	113.95	0.002	0.006	0.003				0.4
Fe-dol-IV	112.92	0.004	0.012	0.005				0.6
Fe-dol-IV	111.71	0.012	0.03	0.013				1
Fe-dol-IV	109.24	0.003	0.007	0.003				0.5
Fe-dol-IV	107.91	0.003	0.009	0.003				0.6
Fe-dol-IV	106.02	0.008	0.017	0.008				1
Fe-dol-IV	104	0.007	0.011	0.005				1
Fe-dol-IV	102.45	0.008	0.02	0.009				0.8
Fe-dol-IV	98.93	0.004	0.011	0.004				0.7
Fe-dol-IV	94.92	0.015	0.03	0.01				1
Fe-dol-IV	90.31	0.03	0.08	0.02				2
Fe-dol-IV	85.18	0.03	0.08	0.02				2
Fe-dol-IV	77.85	0.03	0.08	0.02				2
Fe-dol-IV	68.55	0.015	0.02	0.014				2

Table S4 – Lattice parameters, normalized volume and density of the pure dolomite polymorphs. The errors are reported in a following table.

Structure	<i>P</i> (GPa)	vol <i>V</i> / <i>Z</i>	ρ (g/cm ³)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α (°)	β (°)	γ (°)	<i>V</i> (Å ³)
dolomite	0	106.8	2.867	4.8078		4.8078				320.4
dolomite	3.44	103.6	2.956	4.7805		4.7805				310.6
dolomite	5.54	101.4	3.02	4.7589		4.7589				304
dolomite	7.31	99.8	3.068	4.7468		4.7468				299.6
dolomite	9.5	98.2	3.118	4.7291		4.7291				294.4
dolomite	11.91	96.4	3.176	4.7133		4.7133				289.3
dolomite	14.41	94.8	3.23	4.7012		4.7012				284.5
dol-II	18.16	92.4	3.314	4.714	5.574	7.232	103.57	89.49	91.62	184.6
dol-II	21.27	90.4	3.387	4.695	5.532	7.157	103.35	89.69	91.95	180.8
dol-II	23.82	89.4	3.425	4.697	5.498	7.114	103.22	89.46	92.44	178.7
dol-II	26.44	87.6	3.496	4.686	5.454	7.041	102.77	89.45	92.79	175.3
dol-II	29.4	86.2	3.552	4.672	5.408	6.991	102.47	89.41	93.07	172.2
dol-II	31.12	85.4	3.586	4.668	5.391	6.959	102.32	89.49	93.16	170.8
dol-II	33.59	84.2	3.637	4.657	5.36	6.912	102.05	89.51	93.4	168.4
dol-II	35.74	83.2	3.68	4.649	5.343	6.871	102.03	89.64	93.64	166.6
dol-II	38.46	82.6	3.707	4.645	5.316	6.838	101.78	89.61	93.69	165
dol-II	40.17	82	3.734	4.632	5.291	6.851	101.83	89.48	93.56	164
dol-IIIc	41.51	80	3.828	4.455	11.239	13.714	111.13	91.29	89.77	640.3
dol-IIIc	46.8	78.6	3.896	4.422	11.123	13.659	110.67	91.73	89.78	628.4
dol-IIIc	46.8	78.8	3.886	4.433	11.126	13.662	110.64	91.84	89.92	630.3
dol-IIIc	47.45	78.2	3.916	4.42	11.119	13.613	110.71	91.67	89.75	625.5
dol-IIIc	51.06	78	3.926	4.421	11.106	13.562	110.48	91.66	89.87	623.5
dol-IIIc	51.67	77.8	3.936	4.415	11.101	13.559	110.42	91.64	89.94	622.5
dol-IIIc	53.58	77.4	3.956	4.417	11.065	13.518	110.32	91.74	90.04	619.2
dol-IIIc	55.27	76.8	3.987	4.402	11.033	13.506	110.63	91.87	89.86	613.6
dol-IIIc	55.27	76.4	4.008	4.392	11.03	13.487	110.6	91.66	89.88	611.4
dol-IIIc	56.77	76.6	3.998	4.403	11.033	13.516	111.14	92.15	89.87	612
dol-IIIc	58.46	75.4	4.061	4.38	11.013	13.444	111.41	91.84	89.44	603.4
dol-IIIc	60.8	75.2	4.072	4.384	10.972	13.466	111.51	92.18	89.33	602.2
dol-IIIc	63.16	74	4.138	4.35	10.964	13.334	111.55	91.68	89.37	591.3
dol-IIIc	65.63	73.6	4.16	4.349	10.931	13.306	111.53	91.91	89.34	588.1
dol-IIIc	67.57	73.2	4.183	4.328	10.915	13.32	111.37	91.99	89.45	585.6
dol-IIIc	69.75	72.6	4.218	4.318	10.894	13.261	111.49	91.94	89.36	580.1
dol-IIIc	72.08	72.4	4.229	4.331	10.868	13.245	111.51	92.39	89.36	579.5
dol-IIIc	74.1	72	4.253	4.319	10.85	13.218	111.49	92.49	89.29	575.8
dol-IIIc	76.13	71.6	4.277	4.311	10.827	13.205	111.44	92.68	89.19	573
dol-IIIc	77.98	71.4	4.289	4.316	10.809	13.159	111.48	92.89	89.12	570.5
dol-IIIc	80.49	70.6	4.337	4.294	10.78	13.116	111.48	92.67	88.94	564.3
dol-IIIc	82.08	70.6	4.337	4.296	10.768	13.121	111.28	93.09	89.03	564.7
dol-IIIc	83.9	70.2	4.362	4.291	10.752	13.085	111.37	93.15	88.86	561.3
dol-IIIc	86.46	69.6	4.4	4.282	10.725	13.039	111.3	93.35	88.79	557
dol-IIIc	88.67	69.6	4.4	4.287	10.701	13.009	111.06	93.43	89.13	556
dol-IIIc	88.96	68.6	4.464	4.246	10.684	13.038	111.48	93.51	88.45	549.4
dol-IIIc	89.95	68.8	4.451	4.271	10.691	12.954	111.41	93.24	88.71	549.8
dol-IIIc	92.36	69	4.438	4.291	10.688	12.645	111.28	93.66	88.77	552
dol-IIIc	94.51	68.6	4.464	4.291	10.657	12.913	111.34	93.57	88.93	549
dol-IIIc	97.06	67.8	4.516	4.291	10.647	12.788	111.47	93.23	88.74	543
dol-IIIc	99.78	67.6	4.53	4.284	10.63	12.8	111.54	93.57	89.06	541
dol-IIIc	102.19	67.6	4.53	4.285	10.617	12.75	111.14	93.54	89.15	540

Structure	P (GPa)	$\sigma(a)$	$\sigma(b)$	$\sigma(c)$	$\sigma(\alpha)$	$\sigma(\beta)$	$\sigma(\gamma)$	$\sigma(V)$
dolomite	0	0.0002		0.001				0.3
dolomite	3.44	0.0005		0.003				0.3
dolomite	5.54	0.0005		0.002				0.3
dolomite	7.31	0.0004		0.002				0.3
dolomite	9.5	0.0006		0.003				0.3
dolomite	11.91	0.0005		0.002				0.2
dolomite	14.41	0.0009		0.004				0.2
dol-II	18.16	0.003	0.002	0.004	0.04	0.05	0.04	0.2
dol-II	21.27	0.004	0.002	0.005	0.05	0.06	0.05	0.2
dol-II	23.82	0.003	0.002	0.004	0.04	0.05	0.04	0.2
dol-II	26.44	0.002	0.002	0.004	0.04	0.04	0.04	0.1
dol-II	29.4	0.002	0.001	0.002	0.02	0.03	0.02	0.1
dol-II	31.12	0.002	0.002	0.003	0.03	0.04	0.03	0.1
dol-II	33.59	0.003	0.002	0.004	0.04	0.04	0.04	0.1
dol-II	35.74	0.003	0.002	0.004	0.04	0.06	0.04	0.2
dol-II	38.46	0.004	0.003	0.006	0.06	0.07	0.06	0.2
dol-II	40.17	0.007	0.007	0.011	0.12	0.13	0.12	0.4
dol-IIIc	41.51	0.003	0.006	0.011	0.06	0.06	0.05	0.8
dol-IIIc	46.8	0.002	0.003	0.005	0.03	0.03	0.02	0.4
dol-IIIc	46.8	0.002	0.003	0.005	0.03	0.03	0.02	0.4
dol-IIIc	47.45	0.002	0.004	0.007	0.04	0.04	0.03	0.5
dol-IIIc	51.06	0.003	0.004	0.009	0.05	0.05	0.04	0.6
dol-IIIc	51.67	0.003	0.004	0.01	0.05	0.05	0.04	0.7
dol-IIIc	53.58	0.004	0.006	0.013	0.07	0.07	0.06	0.9
dol-IIIc	55.27	0.002	0.004	0.007	0.04	0.04	0.04	0.5
dol-IIIc	55.27	0.003	0.006	0.009	0.06	0.05	0.05	0.7
dol-IIIc	56.77	0.004	0.006	0.013	0.07	0.08	0.06	1
dol-IIIc	58.46	0.002	0.004	0.007	0.04	0.04	0.04	0.5
dol-IIIc	60.8	0.004	0.007	0.014	0.08	0.08	0.07	1
dol-IIIc	63.16	0.003	0.004	0.009	0.05	0.05	0.04	0.6
dol-IIIc	65.63	0.002	0.004	0.007	0.04	0.04	0.04	0.5
dol-IIIc	67.57	0.003	0.005	0.012	0.06	0.07	0.05	0.8
dol-IIIc	69.75	0.003	0.004	0.01	0.05	0.06	0.05	0.6
dol-IIIc	72.08	0.003	0.005	0.011	0.06	0.06	0.05	0.7
dol-IIIc	74.1	0.003	0.005	0.011	0.06	0.06	0.05	0.7
dol-IIIc	76.13	0.003	0.005	0.01	0.06	0.06	0.05	0.7
dol-IIIc	77.98	0.003	0.005	0.01	0.06	0.06	0.05	0.7
dol-IIIc	80.49	0.003	0.005	0.01	0.06	0.06	0.05	0.7
dol-IIIc	82.08	0.004	0.006	0.014	0.08	0.08	0.07	0.9
dol-IIIc	83.9	0.004	0.006	0.012	0.07	0.07	0.06	0.8
dol-IIIc	86.46	0.005	0.007	0.015	0.09	0.09	0.08	1
dol-IIIc	88.67	0.005	0.008	0.016	0.09	0.01	0.08	1
dol-IIIc	88.96	0.005	0.008	0.016	0.09	0.01	0.08	1
dol-IIIc	89.95	0.004	0.06	0.013	0.08	0.08	0.07	1
dol-IIIc	92.36	0.005	0.007	0.015	0.09	0.09	0.08	1
dol-IIIc	94.51	0.005	0.007	0.015	0.09	0.09	0.08	1
dol-IIIc	97.06	0.006	0.01	0.017	0.1	0.11	0.1	1
dol-IIIc	99.78	0.007	0.012	0.02	0.13	0.13	0.12	1
dol-IIIc	102.19	0.007	0.011	0.02	0.13	0.13	0.11	1

Figure S3 – Normalized volume of dolomite and Fe-dolomite ambient pressure and high pressure polymorphs. It is noticeable that the volume of Fe-dolomite is slightly greater than dolomite, because of the presence of iron in the structure. However, the volume data for Fe-dolomite-IIIb polymorph is sensibly smaller than dolomite-IIIc. This aspect can indicate that Fe could be present in low spin state in the structure of Fe-dolomite-IIIb.

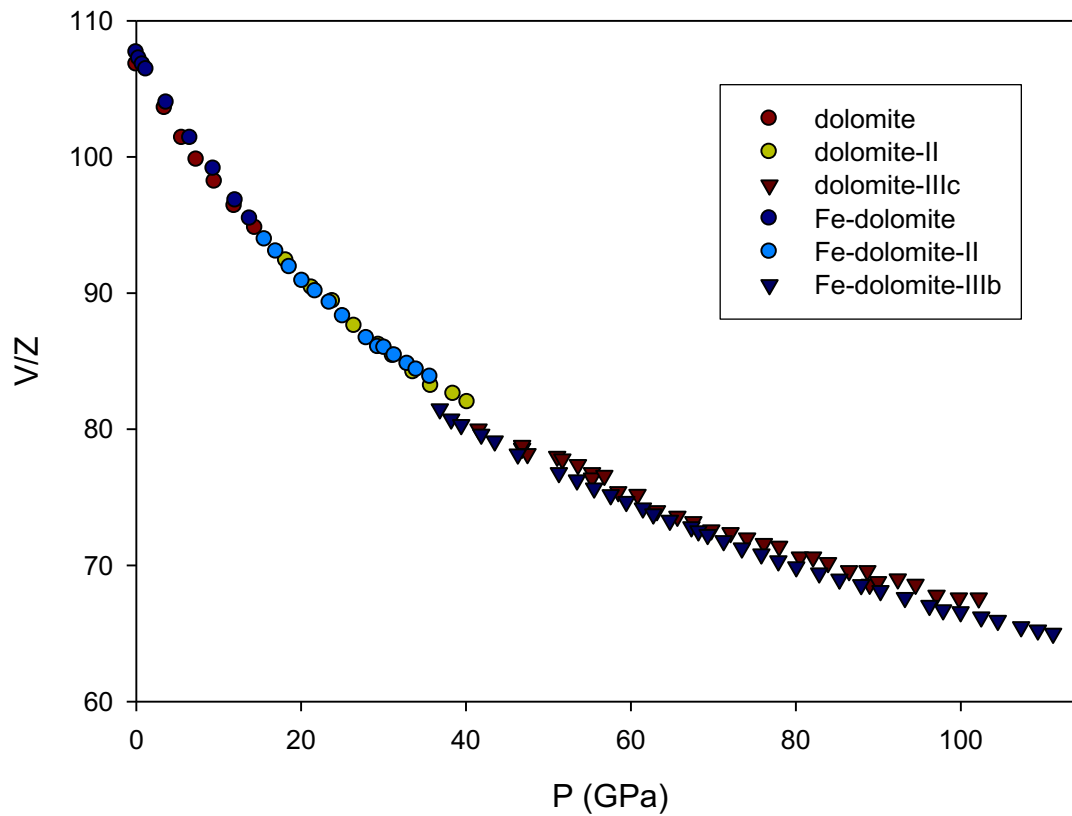


Table S3 - Elastic parameters obtained by 2nd- and 3rd-order Birch-Murnaghan Equation of State fit using the EOS-FIT5.2 program (Angel 2000). The statistical parameters of the fits (*Ru* %, *Rw*%), produced by the EOS-FIT5.2 program, are given.

	2nd-BM-EoS: K_0 (GPa), V_0 (Å³)	3rd-BM-EoS: K_0 (GPa), K', V_0 (Å³)	2nd-BM-EoS: Ru %, Rw%	3rd-BM-EoS: Ru %, Rw%
Fe-dolomite	91.7(10), 323.2(3)	104(2), 1.9(3), 322.9(1)	3.1, 2.9	1.05, 1.01
Fe-dolomite-II	83(3), 216.2(12)	84(2), 3.9(2), 216.2 (fixed)	0.84, 1.08	0.83, 1.09
Fe-dolomite-IIIb	91(9), 2184(18)	91(5), 4.0(3), 2184 (fixed)	0.50, 0.60	0.49, 0.60
Fe-dolomite-IV	150(25), 552(5)	151(14), 3.9(4), 552 (fixed)	5.8, 3.7	5.7, 3.7
Dolomite	95(1), 320.6(3)	95(4), 3.9(6), 320.6(4)	1.08, 1.23	1.13, 1.22
Dolomite-II	76(3), 219(1)	76(2), 4.0(2), 219 (fixed)	0.99, 0.83	0.98, 0.83
Dolomite-IIIc	92(6), 843(13)	91(4), 4.0(2), 843 (fixed)	1.87, 1.99	1.84, 1.99

The unit-cell volume data were fitted to a second- and a third-order Birch-Murnaghan EoS (BM-EoS; Birch 1947; Angel 2000) using the EOS-FIT5.2 program (Angel 2000). The BM-EoS parameters were simultaneously refined using the data weighted by the uncertainties in *P* and *V*. The individual values of V_0 , K_0 and K' are listed in Table S3. For some HP-polymorphs (*i.e.*, Fe-dolomite II, IIIb and IV; Dolomite II and IIIc), the convergence of the 3rd-BM-EoS fit was achieved with the unit-cell volume at room-*P* (*i.e.*, V_0) fixed to the relative value previously refined to a 2nd-BM-EoS fit.