Deposit Items

High pressure experiments

Pressure was increased to 135 GPa in 2 GPa steps. At this maximum pressure the single crystal sample was still in calcite-type R-3c structure (figure 1 and table 1). We performed the first laser heating run at 1800 K for 10 minutes, and after the temperature quench, single crystal data was collected, showing the sample still in R-3c symmetry (table 1). The sample was then further heated at 2650 K for 10 minutes. This temperature is comparable with a low geotherm estimation for the top of the Earth's D'' layer (Anderson, 1982). After temperature quench, diffractions data were collected at 135 GPa. There was a clear indication of sample transformation, with the presence of numerous new single spots, these none continuous powder ring indicated that single crystal domains were present (figure 2-3). Automatic indexing of diffractions failed, but manual observation of diffraction peaks in the reciprocal space with 3D visualizer (Oxford Diffraction, 2008) allowed the identification of at least four different crystals, with random orientation (table 2). Auto-indexing of these diffraction spot series provided two different unit cells, each one observed in two different single crystal domains, reported in table 2 using the conventional crystallographic convention for lattice reduction. Integration of intensity over these four crystals were merged with a second dataset collected with the DAC cell at chi=90° positions, to allow for enough reciprocal space coverage for structure solution. We applied a charge flipping algorithm (Oszlanyi and Suto, 2010) for structure solution. It provided a partial starting model. The missing atoms were located with difference Fourier analysis.

High pressure carbonate structure

The structural model obtained for the carbonate, $Mg_2Fe_2(C_3O_{13})$, was refined against X-ray single crystal diffraction data. HKL-intensity values, corrected for Lorentz-polarization, are reported in the table 3 for the dataset at 135 GPa. The results of refinement of atomic coordinates, isotropic ADP's,

are reported in the article. Statistical agreement indexes are in table 4. No geometrical constraints were applied. Figure 4 shows a plot of the observed and calculated structure factors.

High pressure oxide structure

The structural model obtained for oxide, $Fe_{13}O_{19}$, was refined against X-ray single crystal diffraction data. HKL-intensity values, corrected for Lorentz-polarization, are reported in the table S5 for the dataset at 135 GPa. The results of refinement of atomic coordinates and isotropic ADP's, are reported in the article. No geometrical constraints were applied. Figure 5 and table 6 report a plot of observed and calculated structure factors and statistical agreement indexes.

Equation of state and pressure behavior

We collected single crystal diffraction on decompression, and unit cell parameters were extracted for both the carbonate and oxide structures. We measured pressure with Sm-doped strontium tetraborate fluorescence line and Ne equation of state. The values were in close agreement. In Fig. 6-7 and Table 7 the pressure values reported are derived from EoS of Ne (Fei et al. 2007).

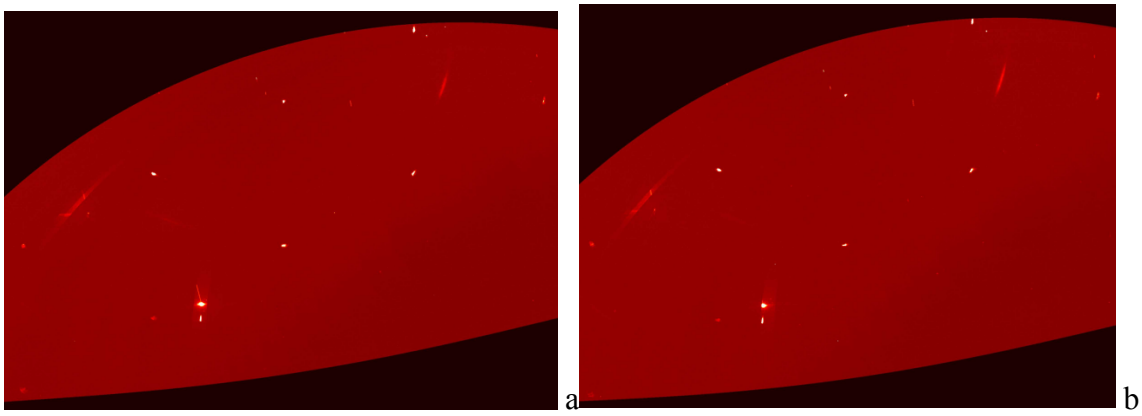

Fig. 1 – Reciprocal space reconstruction (kk2 plane) of single crystal Mg-siderite at 135 GPa before (a) and after (b) heating at 1800 K.

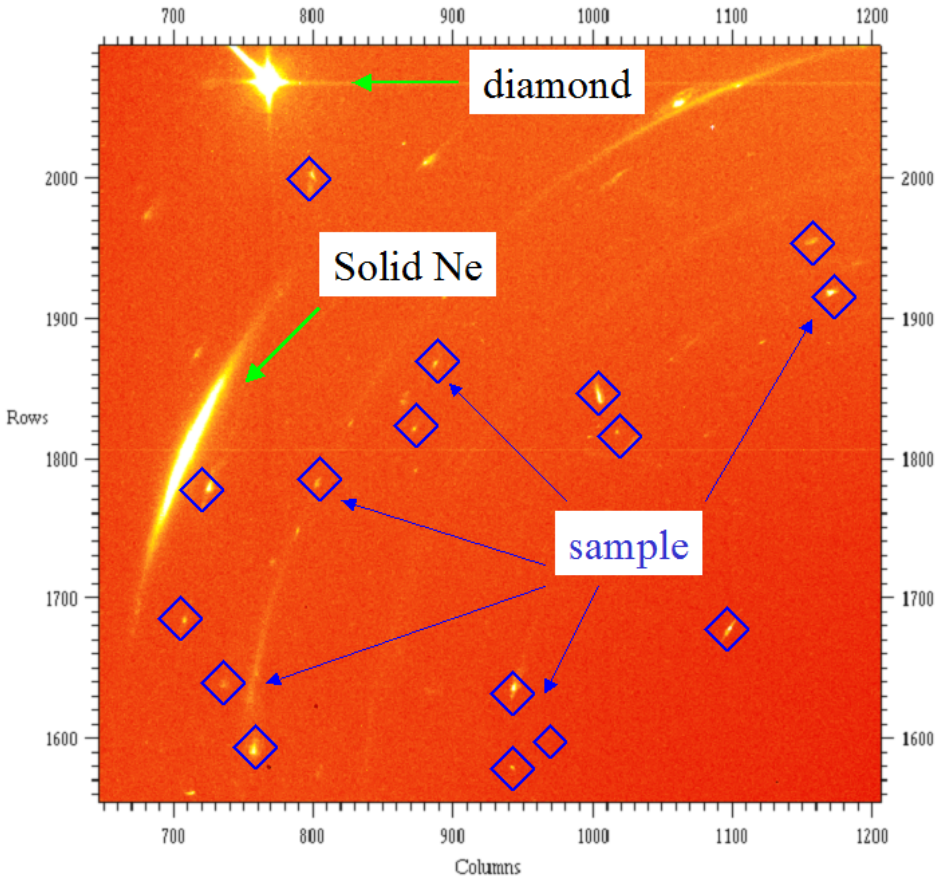

Fig. 2 – Single crystal diffraction spots on 60 deg rotation image of Mg-siderite crystal after heating at 2650 K.

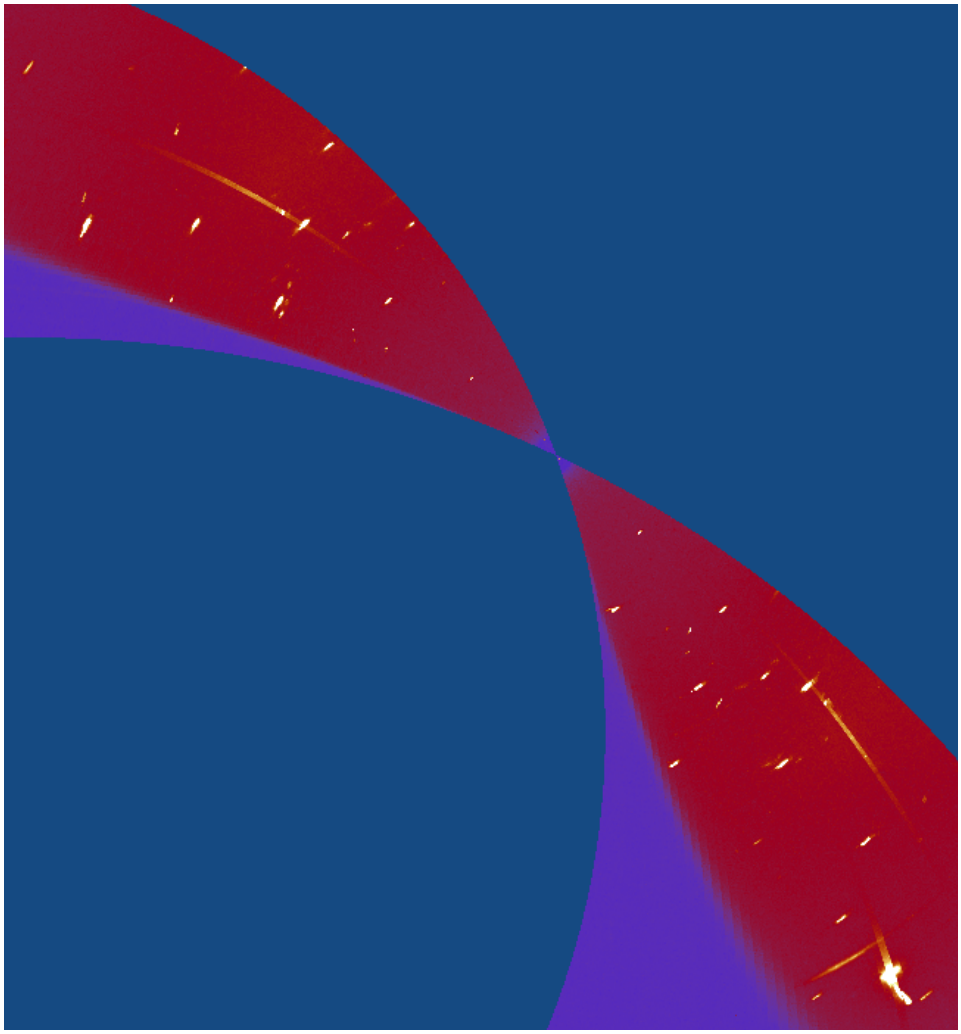

Fig. 3 – Reciprocal space reconstruction (h0l) of the carbonate unwarped from experimental rotation data.

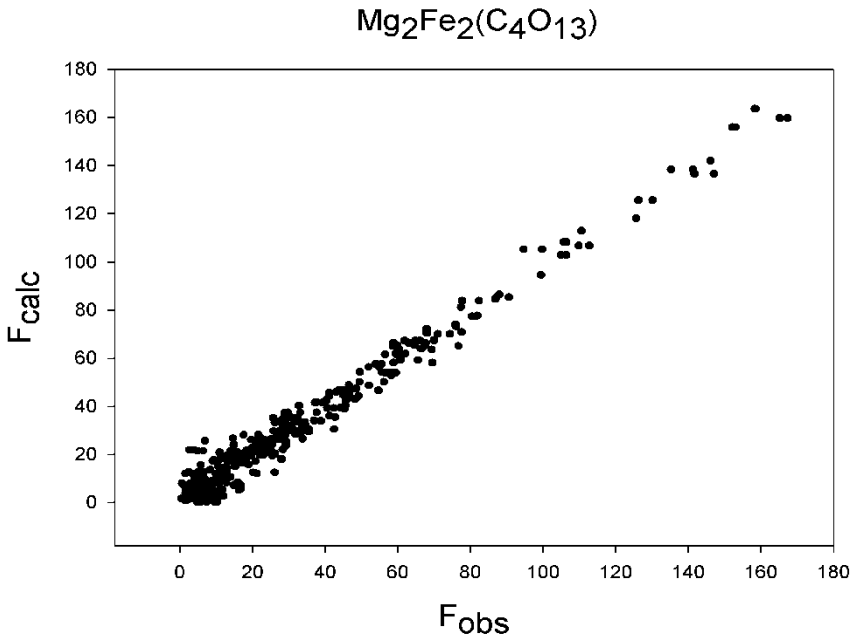

Fig. 4 – Observed (F_{obs}) and calculated (F_{calc}) structure factors for $Mg_2Fe_2(C_4O_{13})$

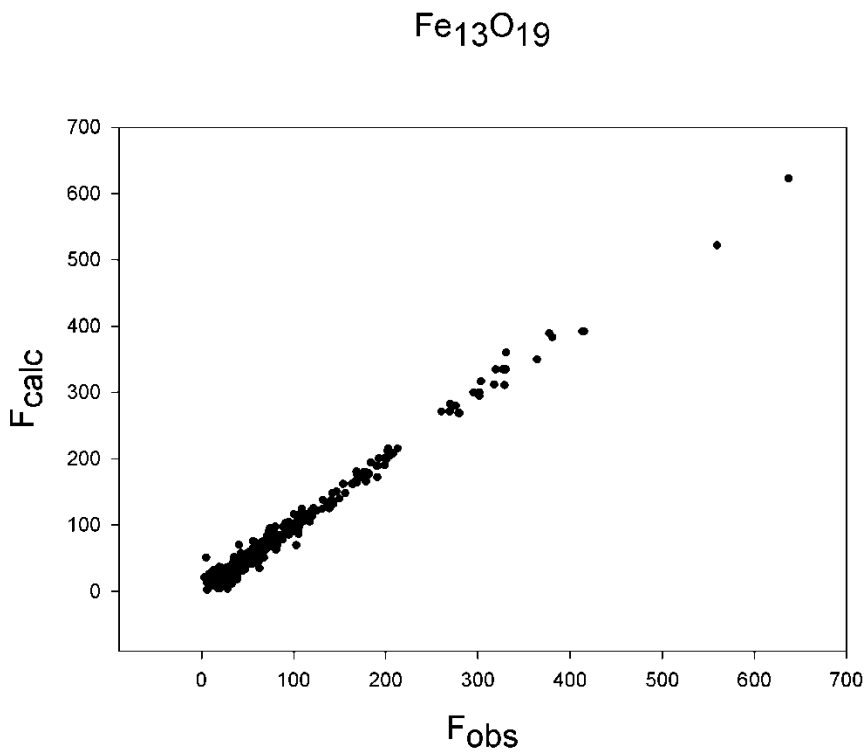

Fig. 5 – Observed (Fobs) and calculated (Fcalc) structure factors for $Fe_{13}O_{19}$

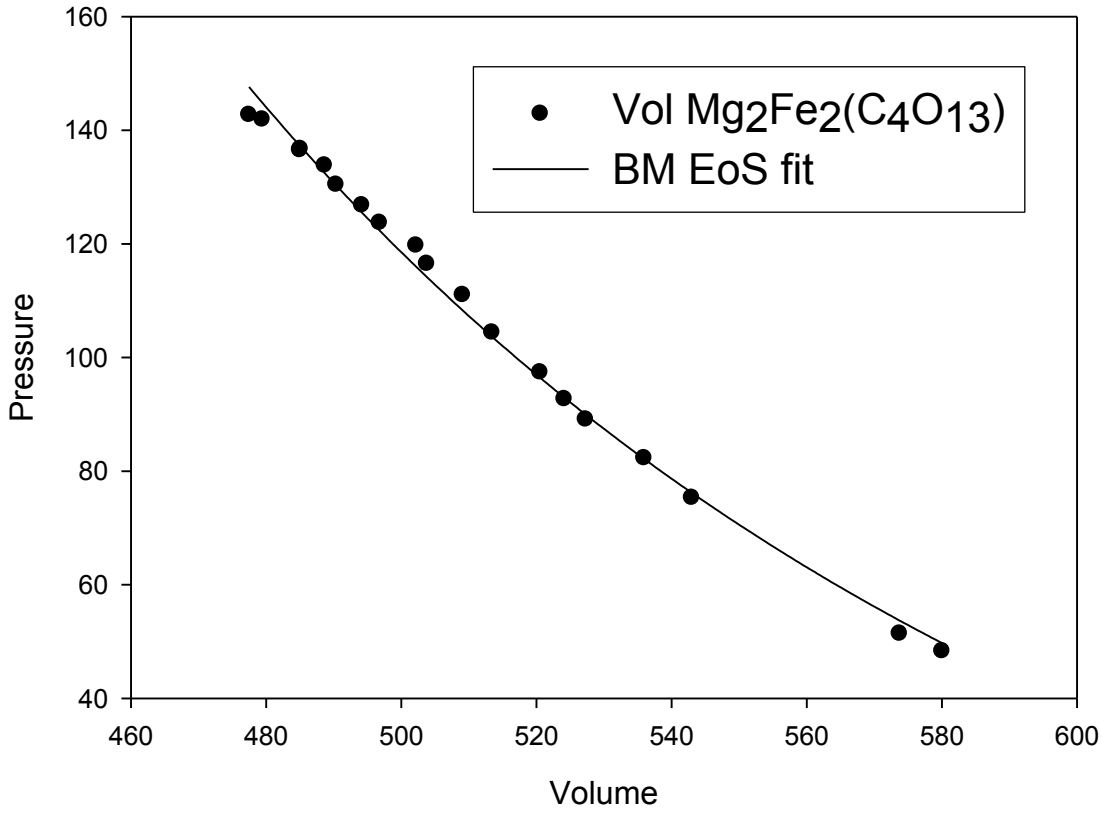

Fig. 6 – PV data for carbonate and Birch-Murnagham Equation of State fit

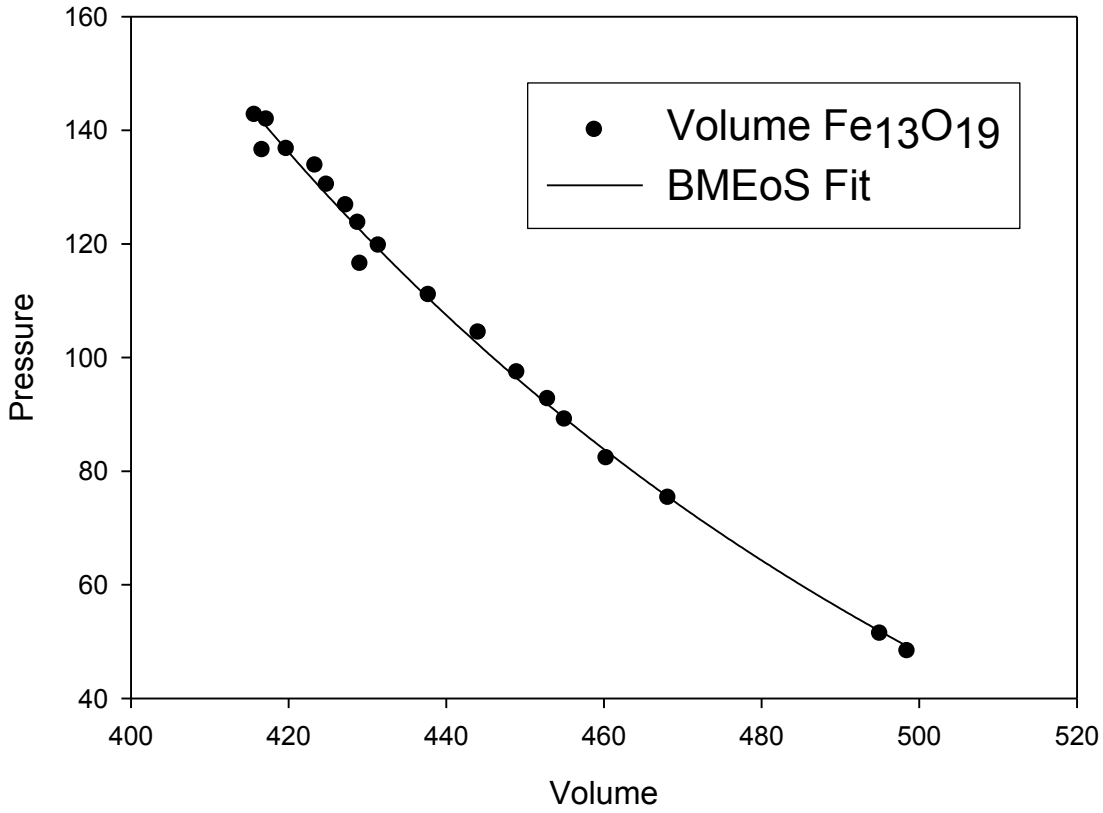

Fig. 7 – PV data for oxide and Birch-Murnagham Equation of State fit

Table 1 – Single crystal refinement of Mg-siderite at 135 GPa before and after heating at 1800 K. Atomic positions in R-3c structure are: Mg-Fe (0, 0, 0); C (0, 0, 0.25); O (x, 0, 0.25)

	(Fe,Mg)CO3 @ 135 GPa before heating	(Fe,Mg)CO3 @ 135 GPa after heating 1800 K
a	4.2319(11)	4.245(2)
c	11.438(6)	11.375(14)
Vol	177.41(17)	177.5(2)
Ox	0.292(1)	0.284(3)
C-O	1.238(5)	1.204(11)
(Fe,Mg)-O	1.783(4)	1.801(8)
R%	6.42	6.36

Table 2 – Lattice parameters for the four crystals indexed after laser heating at 2650 K.

	Crystal 1	Crystal 2	Crystal 3	Crystal 4
a Å	9.823(3)	9.81(3)	19.233(2)	19.26(19)
b Å	3.9022(6)	3.924(5)	2.5820(13)	2.550(12)
C Å	13.154(5)	13.17(4)	9.550(11)	9.55(3)
B (°)	108.02(4)	108.7(4)	118.39(3)	117.3(7)
Volume (Å3)	479.5(3)	480(2)	417.2(5)	416.7(8)
Number of diffractions for UB fit	239	68	136	78

Table 3 – Observed intensities ($|F|^2$) corrected for Lorenz-Polarisation effect for $Mg_2Fe_2(C_4O_{13})$ from data collection at 135 GPa, tabulated as: h,k,l, $|F|^2$,sigma($|F|^2$)

h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)
0	-2	1	3636.14	103.469	2	-2	1	2918.82	125.097	-4	2	-2	7547.39	48.7197	7	-1	-8	15.3776	25.3427
0	-2	2	3531.14	48.4042	-2	2	-2	2088.25	38.8998	-4	2	-3	2.62558	25.328	7	1	-8	6.43063	46.9356
0	2	-2	3858.51	39.9107	2	-2	2	1621.42	30.6063	-4	2	-4	9894.08	63.3081	-7	-1	7	227.373	49.8553
0	-2	3	22.7217	32.9935	-2	2	-3	115.846	25.1628	-4	-4	8	165.492	13.5665	7	1	-7	111.685	60.0567
0	-2	4	20083.7	186.504	2	-2	3	87.9531	35.9271	4	-4	0	4812.54	67.8081	7	-1	-7	161.006	22.3047
0	2	-4	21629.5	176.425	-2	2	-4	11020.1	50.7401	4	-4	2	3085.22	71.1831	-7	-1	6	598.598	38.2293
0	-2	5	2175.5	41.5416	2	-2	4	11330	77.2786	-4	4	-2	2458.22	143.02	7	-1	-6	483.531	19.8338
0	2	-5	1858.18	35.9923	-2	2	-5	357.903	25.3738	-4	4	-3	90.6547	79.3837	-7	-1	5	386.587	61.0211
0	2	-6	265.167	44.3079	2	4	-7	27.1735	110.953	4	-4	3	80.4617	64.9258	-7	-3	11	33.2353	11.8124
0	-2	6	281.3	49.1804	2	4	-6	162.691	151.605	-4	4	-4	3415.48	72.4275	7	3	-9	275.855	167.229
0	2	-7	1001.18	46.562	-2	-4	6	252.776	82.4022	4	-4	4	3547.35	92.4202	7	-3	-4	1421.93	21.7462
0	-2	7	1050.01	93.2545	-2	-4	5	488.248	46.5247	-4	4	-5	450.349	75.0652	-7	3	0	4616.75	53.0278
0	2	-8	1095.8	33.2285	-2	-4	4	5761.13	91.3983	4	-4	5	2.33714	127.889	-7	3	-1	19.3469	54.0078
0	-4	3	685.458	62.4209	2	-4	1	2052.08	54.4622	-4	4	-7	17.6475	90.757	-7	3	-2	685.271	38.6198
0	4	-4	2183.55	172.263	-2	4	-3	17.3634	140.132	-4	4	-8	68.1958	73.2683	-7	3	-4	263.053	46.7627
0	-4	4	2986.29	75.9668	2	-4	4	446.58	40.3165	5	1	-12	212.874	60.3085	8	0	-13	24.0327	53.5402
0	-4	5	6.19652	60.6266	-2	4	-4	805.03	87.8323	5	1	-11	346.743	60.0942	8	0	-12	6020.66	70.1402
0	4	-5	17.9879	133.046	2	-4	5	1098.36	83.3701	-5	-1	10	5996.33	118.188	8	0	-11	26.1744	31.8766
0	4	-6	531.144	83.1034	-2	4	-5	1011.78	69.5178	5	1	-10	4574.08	70.9214	8	0	-10	6610.19	73.2438
0	-4	6	494.055	70.661	2	-4	6	252.924	81.9998	5	1	-9	27.5777	37.6491	8	0	-9	32.5283	56.9207
0	-4	7	953.242	88.2733	-2	4	-6	245.543	72.4143	-5	-1	9	42.846	53.2469	-8	0	9	25.2266	60.0906
0	4	-7	813.743	77.1056	-2	4	-7	38.0582	101.538	-5	-1	8	6786.5	57.0959	-8	0	8	35.1727	44.1109
0	4	-8	121.061	88.256	2	-4	7	68.4293	97.8316	5	1	-8	6045.43	54.6878	8	0	-8	0.35261	38.7811
1	1	-6	3834.75	39.3605	-2	4	-8	3574.64	112.152	5	1	-7	153029	187.812	-8	0	7	110.511	27.8145
-1	-1	6	2843.51	118.871	3	1	-9	723.064	48.1314	-5	-1	7	153922	126.879	-8	0	6	6717.78	172.402
1	1	-5	432.82	19.5284	3	1	-8	387.513	39.5833	5	1	-6	21347.8	73.9122	8	2	-13	1260.36	101.757
-1	-1	5	427.655	33.7835	-3	-1	8	648.17	82.6112	-5	-1	6	21383.2	80.6021	8	2	-12	27.6544	86.689
-1	-1	4	5047.08	40.7552	-3	-1	7	3000.87	46.3268	5	-1	-5	4362.08	25.8102	-8	-2	11	25.2431	71.1353
1	1	-4	5536.48	30.2958	3	1	-7	2697.94	40.3341	5	1	-5	4195.45	51.9287	8	2	-11	35.4816	73.4738
1	1	-3	490.517	15.0631	-3	-1	6	1133.1	39.676	-5	-1	4	5589.06	56.4243	8	2	-10	7601.47	94.8911
-1	-1	3	541.658	17.4576	3	1	-6	1195.19	35.3662	5	3	-10	6253.21	99.9618	-8	-2	10	8216.21	90.2254
1	1	-2	10.434	16.3284	-3	-1	5	4298.07	187.914	-5	-3	9	90.9383	74.5738	8	2	-9	300.738	130.844
-1	-1	2	1.87643	18.056	3	1	-5	3689.49	156.407	5	3	-8	2119.47	95.7834	-8	-2	9	189.034	70.3291
-1	-1	1	50.6606	17.6891	3	1	-4	48065.3	98.0584	-5	-3	8	2024.11	84.5101	8	2	-8	1381.01	164.894
1	1	-1	49.4172	32.3966	-3	-1	4	48526.4	60.3267	5	3	-7	94.9248	137.266	-8	-2	8	1546.89	55.8631
-1	1	0	6472.24	31.6866	-3	-1	3	69.6624	27.9918	-5	-3	7	31.9325	42.0499	-8	-2	7	837.047	80.8151
1	-1	0	6487.82	72.9347	3	1	-3	48.1512	30.1591	-5	-3	6	804.83	68.2345	-8	2	0	541.655	31.4602
-1	1	-1	13.6797	9.21084	-3	1	0	15800.7	36.2829	5	-3	-3	4424.93	48.9656	8	-4	-5	137.724	28.7551
1	-1	1	12.5317	11.3272	3	3	-11	1684.93	88.8254	5	-3	-1	320.477	20.468	-8	4	-2	2714.82	69.7187
-1	1	-2	226.349	9.44198	3	3	-10	278.969	102.729	5	-3	0	327.025	39.172	-8	4	-4	74.2228	76.8306
1	-1	2	294.687	17.7834	-3	-3	10	782.249	80.1714	5	-3	1	595.22	60.5595	9	1	-15	39.2736	74.6186
-1	1	-3	850.046	23.0616	3	3	-9	22.4277	86.1337	-5	3	-1	442.797	40.1997	9	1	-14	55.7333	94.0513
1	3	-11	231.612	65.1539	-3	-3	9	106.965	76.8713	-5	3	-2	2207.36	61.3789	9	1	-13	67.1014	92.0991
-1	-3	10	1804.24	125.133	3	3	-8	1260.4	72.9007	-5	3	-3	304.216	47.2493	9	-1	-12	42.9345	50.0962
1	3	-10	975.265	51.2959	-3	-3	8	850.961	67.6775	-5	3	-4	4894.98	48.9926	9	1	-12	6.06854	98.0072
-1	-3	9	939.691	83.9278	3	3	-7	84.3774	64.3331	-5	3	-5	307.204	57.6978	-9	-1	12	118.412	84.4659
1	3	-9	845.603	65.6793	-3	-3	7	58.2595	55.6005	-5	3	-6	1623.24	59.3678	9	1	-11	10.9558	61.1871
1	3	-8	3986.22	105.719	3	3	-6	3559.37	84.9756	5	-5	0	73.181	59.0281	-9	-1	11	96.0213	70.5582
-1	-3	8	3459.17	99.951	-3	-3	6	3198.11	55.1533	5	-5	1	74.3411	74.38	9	1	-10	3276.44	71.1202
-1	-3	7	2.45421	70.6997	-3	-3	5	44.8734	51.4246	5	-5	2	53.0642	76.964	-9	-1	10	3193.75	77.6158
1	3	-7	28.104	73.7238	3	3	-5	72.6396	115.68	5	-5	3	20.1253	82.3911	-9	-1	9	6.63713	52.8857

1	3	-6	1421.7	69.678	-3	-3	4	16959.1	99.4815	-5	5	-4	1064.67	185.825	9	1	-9	143.898	115.051
-1	-3	6	881.406	56.3082	3	-3	-1	125.484	43.6701	5	-5	4	1365.04	115.42	9	-1	-9	18.89	33.4069
-1	-3	5	2340.49	64.6773	3	-3	0	3656.45	37.4442	5	-5	5	434.378	257.407	-9	-1	8	21.1918	55.2803
1	3	-5	2329.58	57.9211	-3	3	-1	401.268	82.9638	6	0	-10	526.913	44.4608	9	-1	-8	60.2738	59.6687
1	3	-4	1507.7	71.2463	3	-3	1	496.007	37.601	-6	0	8	12718	173.293	-9	-1	7	128.932	46.3395
-1	-3	4	843.474	34.6032	-3	3	-2	294.205	45.7601	6	0	-8	12073.6	57.8297	-9	-1	6	2509.36	64.6669
1	3	-3	1078.6	124.426	3	-3	2	655.81	34.2385	-6	0	7	21.3465	35.4855	-9	1	5	113.788	19.8859
-1	-3	3	2076.96	65.1206	-3	3	-3	3161.13	77.7932	6	0	-7	6.59255	32.6477	-9	1	4	433.585	18.5617
1	-3	1	433.492	54.5047	3	-3	3	2448.7	54.1264	6	0	-6	27998.9	173.825	-9	-3	9	70.5971	10.383
-1	3	-2	93.2365	92.3025	3	-3	4	2350.77	66.777	-6	0	6	27315.2	70.4329	-9	3	0	15.4953	28.4295
1	-3	2	45.7199	41.7569	-3	3	-4	2346.75	63.5168	6	0	-5	21.5442	47.2466	-9	3	-1	219.03	47.1449
-1	3	-3	623.037	51.9181	3	-3	5	8323.61	171.736	-6	0	4	19971.8	147.203	10	0	-15	78.7589	68.4714
1	-3	3	744.141	49.2954	-3	3	-5	5780.78	61.8297	6	2	-13	155.166	78.3033	10	0	-14	3977.88	77.6788
1	-3	4	15946.5	84.6273	-3	3	-6	851.762	44.2836	-6	-2	12	3.87807	84.7035	10	0	-12	119.051	83.5128
-1	3	-4	16942.6	148.29	-3	3	-7	159.426	64.0534	6	2	-12	4.17898	76.9695	10	0	-11	32.4465	51.7943
1	-3	5	1265.96	66.3885	-3	3	-8	1961.49	62.1457	6	2	-11	24.946	96.2276	-10	0	10	33.2166	67.2977
-1	3	-5	1672.39	69.1175	3	-5	1	82.4461	74.2266	-6	-2	11	1.71979	75.6748	-10	0	9	8.41326	50.7622
-1	3	-6	586.729	71.4357	3	-5	2	26.8245	65.1325	6	2	-10	1270.76	92.1319	-10	0	8	14.8732	33.4629
1	-3	6	640.818	65.7319	3	-5	3	25.9306	47.801	-6	-2	10	834.789	78.4194	-10	0	6	18296	60.8643
1	-3	7	191.94	81.9941	3	-5	4	398.595	85.8492	6	2	-9	1243.55	69.198	10	2	-12	210.715	112.654
-1	3	-7	175.305	45.6844	-3	5	-5	1694.15	179.184	-6	-2	9	888.174	61.8436	10	2	-11	3.40664	171.82
1	-3	8	5889.44	199.224	4	0	-7	15.0315	28.227	6	2	-8	4642.91	67.9717	11	-1	-14	1647.03	73.6935
-1	3	-8	3439.65	59.6704	4	0	-6	6785.66	26.7883	-6	-2	8	4613.23	67.3304	11	1	-14	1794.49	82.2971
-1	3	-9	31.1601	76.2781	-4	0	5	6.69053	23.2491	6	2	-7	2169.35	91.0054	11	-1	-13	165.124	68.2946
-1	3	-10	839.68	73.0736	4	0	-4	4994.6	33.8645	-6	-2	7	1394.21	49.9851	11	1	-13	39.5097	85.0814
1	-5	6	0.18509	16.9255	-4	0	4	3701.44	53.3813	-6	-2	6	9945.07	101.8	-11	-1	13	99.4519	98.1925
2	0	-4	12225.7	80.9632	4	0	-3	4.69425	29.5066	6	2	-6	8965.26	142.458	11	-1	-12	41.2507	46.2864
-2	0	2	649.851	8.72575	-4	0	3	3.24081	18.145	-6	-2	5	47.8705	72.9312	-11	-1	12	24.018	82.6093
2	0	-2	620.129	8.23281	4	2	-13	158.138	72.8892	-6	2	1	7.63513	15.2585	11	1	-12	194.932	136.89
2	2	-11	663.254	65.6644	4	2	-12	3461.14	90.8544	6	-4	-2	1179.7	43.3309	11	-1	-11	22.4984	64.3138
2	2	-10	345.683	60.275	-4	-2	12	4834.91	269.615	6	-4	-1	18.4287	53.5465	-11	-1	10	4244.01	76.8547
-2	-2	10	638.608	227.61	-4	-2	11	474.166	100.117	6	-4	0	408.178	54.6297	-11	-1	8	284.267	38.6827
2	2	-9	561.877	50.611	4	2	-11	340.147	51.8622	6	-4	1	3391.95	86.455	-11	1	6	32.6861	22.4768
-2	-2	9	584.879	84.2424	4	2	-10	736.714	48.3868	-6	4	-2	22.7959	101.59	12	0	-14	725.824	73.2611
-2	-2	8	11199.5	85.9262	-4	-2	10	1053.26	76.9298	-6	4	-3	102.852	58.4634	-12	0	10	1408.92	69.8313
2	2	-8	11332	78.1887	4	2	-9	3.32468	58.0312	-6	4	-4	680.66	73.0258	-12	0	9	32.5426	56.7329
2	2	-7	309.76	37.5312	-4	-2	9	74.5426	55.8787	-6	4	-5	36.1878	85.096	-12	0	8	331.786	47.5176
-2	-2	7	466.553	57.7384	4	2	-8	2425.64	81.35	-6	4	-6	752.663	88.5513	-12	0	7	1.30514	37.435
2	2	-6	1922.58	60.2785	-4	-2	8	1688.54	46.2031	-6	4	-7	468.869	73.2371	-13	-1	13	477.976	93.3922
-2	-2	6	2002.76	46.8344	-4	-2	7	48.802	45.4363	7	1	-14	4589.78	94.4613	-13	-1	12	335.777	92.7919
2	2	-5	1141.76	54.2452	4	2	-7	98.6506	72.1785	7	1	-13	24.0603	54.9641	-13	-1	10	1821.4	71.5003
-2	-2	5	680.177	44.5163	4	2	-6	220.199	47.8025	-7	-1	12	1075.76	187.777	-13	1	6	943.328	29.5475
-2	-2	4	25060.7	74.0571	-4	-2	6	280.046	37.834	7	1	-12	746.413	41.5867	-14	0	12	113.472	78.264
2	2	-4	25150	76.2161	4	2	-4	19.0857	101.15	-7	-1	11	127.376	79.8131	-14	0	11	1.53844	68.4243
-2	-2	3	19124	97.1762	4	-2	-2	7742.63	33.8405	7	1	-11	105.42	52.1624	-14	0	10	661.612	70.6896
2	2	-3	18516.1	102.436	4	-2	-1	122.686	12.3439	7	1	-10	4550.34	89.4471	-14	0	9	17.4054	33.8827
2	-2	-1	1179.93	24.9082	-4	2	0	23166.7	113.147	-7	-1	10	3585.54	80.0039					
2	-2	0	4176.71	40.7298	4	-2	0	23431.3	56.1745	7	1	-9	933.666	79.4495					
-2	2	-1	3082.33	80.989	-4	2	-1	166.722	34.1932	7	-1	-9	925.063	29.2434					

Table 4 – R factors for single crystal structure refinement of $Mg_2Fe_2(C_4O_{13})$ on dataset collected at 135 GPa.

R(F>3σF)	9.07
R(all)	12.09
Refined parameters	45
N. reflections	368 (253 F>3σF)

Table 5 – Observed intensities ($|F|^2$) corrected for Lorenz-Polarisation effect for $Fe_{13}O_{19}$ from data collection at 135 GPa, tabulated as: h,k,l, $|F|^2$,sigma($|F|^2$)

h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)	h	k	l	*I*	sig(*I*)
0	0	2	131.895	10.4792	3	-1	-6	3190.25	41.0917	-6	0	6	1744.48	45.3054	-10	-2	4	445.02	36.668
0	0	-2	122.554	13.336	-3	-1	5	205.672	37.4464	6	0	-6	1740.29	34.4255	-10	-2	3	298.039	36.1724
0	0	3	150.749	17.5373	3	-1	-5	198.134	30.8339	-6	0	5	336.108	39.4307	11	1	-11	2.63408	18.7699
0	0	-3	100.302	22.8885	-3	-1	4	10818.3	54.6771	6	0	-5	482.954	27.0495	-11	-1	10	554.964	74.3837
0	0	4	152.977	24.375	-3	-1	3	1484.33	33.8385	6	0	-4	3.67384	25.4686	11	1	-9	1003.72	73.4364
0	0	5	313.624	35.4323	-3	-1	2	7611.35	37.8505	-6	-2	3	169.494	36.1048	-11	-1	9	1140.1	74.1782
0	0	6	1038.47	49.5411	-3	-1	1	586.693	19.2647	-6	-2	2	21.4257	30.4494	-11	-1	8	20.3974	64.9772
0	0	7	2857.12	71.8322	3	1	3	14502.9	37.9043	7	-1	-11	165.692	73.0307	-11	-1	7	511.385	58.8553
0	0	8	457.683	80.97	3	1	4	2154.25	32.3899	7	-1	-10	3183.55	80.5077	11	1	-7	566.179	72.6129
0	0	9	626.862	83.1577	3	1	5	1173.22	30.9517	-7	-1	10	2786.76	86.3451	-11	-1	6	1185.11	59.1173
0	0	10	2844.57	90.5056	3	1	6	656.473	36.1044	7	-1	-9	64.1759	58.1793	11	1	-6	1717.98	51.4197
0	-2	-5	223.616	31.1653	3	1	7	1375.63	44.6539	7	1	-8	1087.05	76.8402	11	1	-5	10078.8	59.46
0	-2	-6	373.173	37.4943	3	1	8	1930.69	55.4067	7	-1	-8	1220.52	50.6131	11	1	-4	381.483	32.3284
0	-2	-7	1185.57	60.163	3	1	9	298.576	61.7165	-7	-1	7	3088.83	60.6647	11	1	-3	7286.68	45.2564
0	-2	-8	106.808	49.551	3	1	10	3640.98	76.7874	7	1	-7	2924.62	71.4411	-11	-3	6	397.81	65.1338
0	-2	-9	264.662	59.9539	3	1	11	196.922	78.2141	-7	-1	6	449.737	45.0769	-11	-3	5	1986.44	57.1778
0	-2	-10	1451.35	80.2921	-4	0	11	6.88468	59.5907	7	1	-6	397.394	48.9024	-11	-3	4	37.434	44.7159
-1	1	11	1155.12	88.3393	-4	0	10	735.855	68.8526	7	1	-5	4338.29	45.8265	-11	-3	3	1478.2	45.5456
-1	1	10	100.341	75.754	4	0	-10	664.418	101.384	-7	-1	5	4252.42	45.2333	12	0	-9	108.038	58.094
1	-1	-10	95.3097	97.2436	-4	0	9	394.757	68.322	7	1	-4	3609.42	42.122	12	0	-8	1002.21	50.0795
1	-1	-9	574.577	76.6313	-4	0	8	17255.6	85.8354	-7	-1	4	3656.6	36.5583	-12	-2	8	312.644	67.094
-1	1	9	778.733	62.7885	4	0	-8	17094.5	92.5042	7	1	-3	4203.03	40.5065	-12	-2	7	211.122	56.2509
1	-1	-8	1095.26	56.6295	4	0	-6	323.351	44.1056	-7	-1	3	4108.55	32.5576	12	2	-7	102.375	82.9958
-1	1	8	879.737	56.3032	-4	0	6	303.073	33.9816	7	1	-2	985.686	22.0336	-12	-2	6	42.3604	57.1855
1	-1	-7	1110.38	49.1339	4	0	-5	7856.99	53.7816	7	1	-1	13263.8	44.4425	12	2	-6	77.4502	73.8237
-1	1	7	648.645	55.4977	-4	0	5	7784.07	44.3259	7	1	4	657.418	30.4903	-12	-2	5	75.0288	49.0066
1	-1	-6	447.952	49.5966	-4	0	4	928.055	25.2783	7	1	5	1020.62	38.9131	12	2	-4	20.0709	54.3597
1	-1	-5	2907.96	31.7531	4	0	-4	1043.78	23.5097	7	1	6	167.633	52.145	12	2	-3	18.4103	45.2033
1	-1	-4	34.7619	22.2199	4	0	-3	34.8612	17.2523	-7	-3	0	595.971	23.6796	13	1	-11	125.086	15.4241
-1	-1	-3	459.465	17.8692	4	-2	-11	0.97704	79.7342	-8	0	11	110.33	83.9234	-13	-1	10	621.609	97.3722
-1	-1	-4	9200.87	44.2674	4	-2	-10	366.157	83.2637	-8	0	10	752.861	80.8575	13	1	-9	3712.83	106.106
1	1	5	2366	36.4332	4	-2	-9	149.507	54.7755	8	0	-10	535.765	74.5538	-13	-1	9	3928.93	95.5948
-1	-1	-5	2713.52	34.0224	-4	-2	-3	6.04746	10.057	-8	0	9	781.698	78.0322	13	1	-8	225.039	74.2731
-1	-1	-6	43.6794	45.2731	-4	-2	-4	124.781	23.779	8	0	-9	838.815	88.0932	13	1	-7	3309.97	62.1352
1	1	6	27.4917	38.076	5	-1	-11	518.604	77.6486	8	0	-8	59.6516	53.8788	13	1	-6	1322.86	48.4083
1	1	7	2437.52	48.9349	5	-1	-10	677.188	82.3812	-8	0	8	85.3955	59.7646	13	1	-4	2676.3	39.3941
-1	-1	-7	2013.11	67.157	-5	-1	10	1062.26	86.5287	8	0	-7	1864.16	46.4333	-13	-3	8	57.2991	72.7957
1	1	8	605.67	48.8863	5	-1	-9	847.67	72.2844	8	0	-6	8.05855	33.0994	-13	-3	7	937.808	71.0704
1	1	9	184.112	55.2346	-5	-1	9	549.996	80.2363	8	0	-5	485.17	33.5851	-13	-3	6	239.227	62.6172
1	1	10	378.058	69.6558	5	-1	-8	1441.14	54.4643	-8	-2	7	535.555	75.7724	14	0	-10	149.137	66.1944
1	1	11	235.768	75.8424	-5	-1	8	1416.02	79.2164	-8	-2	6	14.9331	63.889	-14	-2	9	574.825	86.025
-2	0	10	354.843	76.6257	-5	-1	7	415.993	62.2794	-8	-2	5	119.669	51.2256	14	2	-8	25.4499	88.4769
-2	0	9	355.006	66.4759	5	-1	-7	394.685	42.5311	-8	-2	4	204.163	45.0708	-14	-2	8	57.6722	72.3907
-2	0	8	1130.56	62.7925	-5	-1	6	8727.59	81.7264	-8	-2	3	14256.9	58.4168	14	2	-7	13.8254	73.934
2	0	-8	640.129	81.9059	5	-1	-6	9106.22	58.1284	-8	-2	2	218.98	25.91	14	2	-6	933.318	61.9781
2	0	-7	176.529	59.0761	5	1	-5	350.816	52.9642	-8	-2	1	27.8595	20.8089	14	2	-5	32.8325	50.6534
-2	0	7	231.064	49.3335	-5	-1	5	369.52	49.6212	9	-1	-10	753.653	68.8569	14	2	-4	7.49636	37.6112
-2	0	6	277.054	40.7669	-5	-1	4	10182.9	58.1031	-9	-1	10	901.338	73.0099	14	2	-3	300.319	32.6896
2	0	-6	268.921	46.0497	5	1	-4	10899.2	58.9137	9	1	-9	10.4576	89.1035	14	2	-2	10947	83.6798

-2	0	5	2038.06	36.8091	-5	-1	3	7254.41	44.0795	-9	-1	8	632.749	56.5905	14	2	-1	501.326	18.6429
2	0	-5	2050.1	32.9846	5	1	-3	6785.96	43.8935	9	1	-8	542.396	57.2574	15	1	-9	91.2679	75.7048
-2	0	4	40589.3	78.2016	-5	-1	2	102.479	16.5691	-9	-1	7	224.126	47.6895	15	1	-8	300.903	63.6594
2	0	-4	40637.6	78.4559	5	1	-2	74.44	22.0505	9	1	-7	159.64	52.3254	15	1	-7	1023.21	53.6325
-2	0	2	5.45371	10.0242	5	1	-1	3985.02	22.0949	-9	-1	6	182.528	42.4492	-15	-3	8	113.886	83.5883
2	0	-2	3.60353	9.66216	-5	-1	1	4038.28	18.3235	9	1	-6	120.694	50.7909	-15	-3	7	212.004	79.9188
2	-2	-11	468.187	77.0606	5	1	2	4084.16	22.7425	9	1	-5	4536.48	123.291	16	2	-7	28.5639	60.2245
2	-2	-10	178.007	67.566	5	1	3	3382.39	33.1346	-9	-1	5	4106.28	66.7897	16	2	-6	9101.48	75.142
2	-2	-9	200.889	69.782	5	1	4	3132.61	37.8896	9	1	-4	54.7738	33.9224	16	2	-5	69.6331	51.3106
2	-2	-8	438.083	55.6203	5	1	5	567.05	41.9835	-9	-1	4	38.9661	39.2996	16	2	-4	41.368	48.5809
2	-2	-7	17.4464	41.6413	5	1	6	2241.16	47.247	9	1	-3	3283.18	30.9888	16	2	-2	110.863	32.3524
-2	-2	-4	31.3822	22.0763	5	1	7	317.13	52.2231	9	1	-2	2842.77	29.6714	16	2	-1	9.40931	22.6532
-2	-2	-5	40.9005	39.8851	5	1	9	434.391	68.3657	-9	-3	2	433.502	35.4902	16	2	0	288.028	15.5025
-2	-2	-6	1311.24	35.6931	5	1	10	732.647	69.626	-9	-3	1	828.06	23.9532	17	1	-9	80.6025	73.4146
-2	-2	-7	37.0497	50.1399	-6	0	11	123.025	79.6738	-10	0	11	20.5058	103.055	17	1	-8	1422.61	63.1947
3	-1	-11	899.95	95.2038	6	0	-10	494.941	77.3645	10	0	-10	59.7522	88.8796	18	2	-8	31.7892	67.8412
-3	1	11	892.598	100.839	-6	0	10	668.959	72.4574	10	0	-8	779.275	55.0661	18	2	-6	152.219	77.89
3	-1	-10	328.221	74.9255	6	0	-9	1425.84	67.4141	10	0	-7	31328.5	97.6084	18	2	-5	11.6036	59.868
-3	1	10	120.47	81.4206	-6	0	9	1557.59	63.6038	10	0	-6	1077.17	33.3163	18	2	-4	107.971	47.1249
3	-1	-9	3947.56	69.7999	6	0	-8	1232.17	64.6251	-10	-2	8	249.666	68.5635	18	2	-3	564.02	40.8946
3	-1	-8	150.064	66.2683	-6	0	8	1199.81	55.5634	-10	-2	7	10728	86.1194	20	2	-8	73.8605	85.4538
3	-1	-7	1130.51	51.363	6	0	-7	38.5744	54.5205	-10	-2	6	47.2621	52.472	20	2	-7	31.5194	78.1147
-3	-1	6	3099.6	51.7836	-6	0	7	49.0697	45.5573	-10	-2	5	68.231	44.0867	22	2	-8	32.5416	88.8706

Table 6 - R factors for single crystal structure refinement of $Fe_{13}O_{19}$ on dataset collected at 135 GPa.

R(F>3σF)	4.99
R(all)	7.25
Refined parameters	48
N. reflections	283 (206 F>3σF)

Table 7 – Unit cell parameters of $Mg_2Fe_2(C_4O_{13})$ and $Fe_{13}O_{19}$ determined with single crystal diffraction on decompression from 135 GPa. Errors are in the 0.001-0.01 range for lattice parameters; 0.05 for angle and 0.05-0.1 for volume data.

	$Mg_2Fe_2(C_4O_{13})$						$Fe_{13}O_{19}$					
P (Gpa)	a	b	C	beta	vol	ρ (g/cm^3)	a	b	c	beta	vol	ρ(g/cm^3)
141.9	9.822	3.9023	13.154	108.02	479.44	5.768	19.233	2.582	9.55	118.39	417.21	8.199
142.7	9.808	3.894	13.138	107.9	477.48	5.792	19.219	2.5582	9.53	117.48	415.69	8.229
136.5	9.886	3.9158	13.176	108.04	484.99	5.702	19.258	2.5718	9.543	118.17	416.66	8.21
136.7	9.883	3.9099	13.19	107.87	485.09	5.701	19.295	2.567	9.554	117.5	419.74	8.15
133.8	9.925	3.9171	13.204	107.84	488.65	5.659	19.327	2.5889	9.601	118.2	423.37	8.08
130.4	9.952	3.9171	13.21	107.78	490.37	5.64	19.367	2.5895	9.611	118.19	424.83	8.052
126.8	9.998	3.9199	13.233	107.66	494.18	5.596	19.38	2.595	9.635	118.14	427.28	8.006
123.7	10.024	3.9257	13.253	107.71	496.81	5.566	19.429	2.5963	9.643	118.17	428.81	7.977
119.7	10.08	3.9358	13.283	107.64	502.2	5.507	19.488	2.6	9.656	118.14	431.43	7.929
116.5	10.1	3.9465	13.269	107.72	503.8	5.489	19.484	2.5913	9.635	118.11	429.08	7.972
111	10.136	3.9562	13.326	107.7	509.08	5.432	19.626	2.6055	9.701	118.06	437.76	7.814
104.4	10.176	3.9637	13.356	107.62	513.44	5.386	19.748	2.6134	9.747	118.02	444.07	7.703
97.4	10.234	3.9835	13.397	107.61	520.56	5.312	19.839	2.6209	9.775	117.95	448.98	7.619
92.7	10.268	3.9946	13.405	107.58	524.15	5.276	19.924	2.6257	9.799	117.94	452.88	7.553
89.1	10.288	4.0048	13.425	107.58	527.3	5.245	19.981	2.6262	9.81	117.88	455.02	7.518
82.3	10.348	4.03	13.479	107.55	535.94	5.16	20.071	2.6348	9.842	117.82	460.32	7.431
75.3	10.402	4.0509	13.513	107.52	542.99	5.093	20.184	2.6494	9.892	117.75	468.14	7.307
51.4	10.628	4.145	13.642	107.31	573.75	4.82	20.447	2.7068	10.126	117.96	495.02	6.91
48.3	10.672	4.1659	13.676	107.45	580.03	4.768	20.52	2.7092	10.159	118.04	498.47	6.863

Table 8 – Refined total Mg occupancy in $Mg_2Fe_2(C_4O_{13})$ obtained from the twelve single crystal refinements form experimental data in the pressure range 75-140 GPa. The average value is 0.39(6), and the consequent stoichiometry of carbonate is $Mg_{1.57}Fe_{2.43}(C_4O_{13})$

Mg occupancy
0.28(3)
0.32(3)
0.31(3)
0.41(3)
0.34(4)
0.39(4)
0.46(2)
0.48(3)
0.41(3)
0.38(2)
0.46(3)
0.47(2)