

Table S 1 Results of the crystal structure refinement based on single-crystal X-ray diffraction data for skiagite-majorite garnets with the composition Ski_{76.6}Maj_{23.4} (run S6073)

N of the run	S6073						
Crystal system	cubic						
Space group	$1a\bar{3}d$						
Z	8						
P, GPa	4.03(5)	8.6 (5)	11.8(6)	14.8(7)	17.6(3)	21.3(2)	26.45(1)
a (Å)	11.6194(3)	11.5171(2)	11.4665(3)	11.4126(2)	11.3700(6)	11.3143(12)	11.2405(3)
V (Å ³)	1568.74(6)	1527.83(7)	1507.62(7)	1486.46(5)	1469.89(4)	1448.38(2)	1420.22(4)
FeO ₈ , V ₀ , Å ³	20.5332	19.7703	19.4157	19.0478	18.7728	18.3817	17.9276
(Fe,Si)O ₆ , V ₀ , Å ³	10.1701	9.9449	9.8257	9.7316	9.6324	9.5376	9.4057
SiO ₄ , V ₀ , Å ³	2.1872	2.1687	2.1579	2.1402	2.1283	2.1122	2.0814
F(000)	2122	2122	2118	2122	2122	2122	2122
Theta range for data collection(°)	2.51/20.71	2.53/20.45	2.48/19.97	2.55/20.57	2.56/20.67	2.58/20.78	2.58/20.07
Index ranges	-12 < h < 10	-18 < h < 17	-18 < h < 17	-18 < h < 17	-13 < h < 11	-13 < h < 11	-16 < h < 18
	-19 < k < 18	-18 < k < 18	-17 < k < 18	-17 < k < 18	-18 < k < 18	-18 < k < 18	-16 < k < 16
	-19 < l < 17	-10 < l < 12	-12 < l < 11	-11 < l < 12	-18 < l < 16	-18 < l < 16	-9 < l < 14
No.of measured, independent, and observed[I>2s(I)] reflections	2027/289/224	1900/281/205	1956/279/212	1971/278/217	1905/276/205	1855/270/203	1647/258/169
R _{int}	4.46	4.02	5.72	5.62	3.31	3.17	4
No.of parameters/restraints/ constraints	17/0/2						

Final R indices [$I > 3\sigma(I)$] R_F/wR_F	0.0421/0.0576	0.0483/0.0580	0.0376/0.0466	0.0351/0.0465	0.0393/0.0517	0.0395/0.0522	0.0403/0.0452
R indices (all data) R_F/wR_F	0.0512/0.0597	0.0597/0.0607	0.0476/0.0497	0.0435/0.0488	0.0498/0.0540	0.0505/0.0551	0.0597/0.0476
Largest diff. peak /hole ($e / \text{\AA}^3$)	0.91/0.87						

N of the run	S6073						
Crystal system							
Space group							
Z							
P, GPa	14.0(5)	16.78(55)	22(1)	27.7(5)	34.85(5)	40.56(12)	44.54(67)
a (\AA)	11.4254(2)	11.3754(5)	11.2909(8)	11.2109(5)	11.1202(6)	11.0574(5)	11.015(4)
V (\AA^3)	1491.47(5)	1471.9(1)	1439.42(18)	1409.03(11)	1375.11(13)	1351.95(11)	1336.52(8)
FeO ₈ , V ₀ , \AA^3	19.1122	18.7803	18.2215	17.7552	17.1925	16.8509	16.6429
(Fe,Si)O ₆ , V ₀ , \AA^3	9.7264	9.6747	9.4936	9.3180	9.1579	9.0184	8.9068
SiO ₄ , V ₀ , \AA^3	2.1542	2.1285	2.1015	2.0719	2.0386	2.0149	2.0057
F(000)					2122	2122	2122
Theta range for data collection(°)	2.55/20.22	2.56/20.66	2.58/20.82	2.6/20.26	2.62 20.44	2.64/20.56	2.64/20.61
Index ranges	-17 < h < 14	-12 < h < 12	-12 < h < 12	-12 < h < 11	-12 < h < 11	-14 < h < 17	-14 < h < 17
	-17 < k < 14	-18 < k < 15	-17 < k < 15	-17 < k < 14	-17 < k < 14	-14 < k < 17	-14 < k < 17
	-12 < l < 14	-17 < l < 15	-14 < l < 18	-14 < l < 17	-14 < l < 17	-12 < l < 11	-12 < l < 11
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	1781/268/205	1713/274/177	1665/269/142	1548/257/167	1524/253/152	1509/251/155	1545/254/166

R _{int}	2.17	5.3	6.2	6.1	5.85	6.81	7.19
No.of parameters/restraints/ constraints	17/0/2						
Final R indices [I>3σ(I)]R _F /wR _F	0.0489/0.0609	0.0589/0.0701	0.0741/0.0764	0.0692/0.0755	0.0655/0.0715	0.0664/0.0718	0.0697/0.0787
R indices (all data) R _F /wR _F	0.0582/0.0624	0.0735/0.0732	0.0995/0.0804	0.0879/0.0798	0.0889/0.0745	0.0831/0.0741	0.0839/0.0804
Largest diff. peak /hole (e / Å ³)	0.91/0.87						

N of the run	S6073						
Crystal system	cubic						
Space group	$Ia\bar{3}d$						
Z	8						
P, GPa	52.15(3)	57.92(4)	62.2(8)	66.73(85)	71.55(18)	77.2(5)	80.99(42)
a (Å)	10.9287(8)	10.8128(15)	10.7485(7)	10.7125(11)	10.6679(8)	10.6373(12)	10.6150(15)
V (Å ³)	1305.27(15)	1264.2(3)	1241.78(15)	1229.34(22)	1214.05(16)	1203.6(2)	1196.1(3)
FeO ₈ , V ₀ , Å ³	16.2218	15.8093	15.5801	15.3870	15.1782	14.9626	14.8935
(Fe,Si)O ₆ , V ₀ , Å ³	8.6497	8.0129	7.8020	7.6927	7.6053	7.5959	7.4979
SiO ₄ , V ₀ , Å ³	1.9894	1.9873	1.9660	1.9679	1.9427	1.9409	1.9474
F(000)	2122	2122	2122	2122	2122	2122	2122
Theta range for data collection(°)	2.7/20.56	2.7/20.6	2.7/20.73	2.7/20.74	2.73/20.83	2.73/20.57	2.75/20.67
Index ranges	-12 < h < 10	-14 < h < 16	-13 < h < 17	-14 < h < 17	-16 < h < 14	-11 < h < 13	-9 < h < 13
	-17 < k < 14	-11 < k < 12	-13 < k < 16	-14 < k < 16	-17 < k < 14	-14 < k < 17	-14 < k < 17
	-14 < l < 17	-11 < l < 14	-12 < l < 11	-12 < l < 11	-11 < l < 12	-16 < l < 13	-16 < l < 13
No. of measured, independent, and observed [I > 3σ(I)] reflections	2736/239/192	1405/234/131	1327/233/177	1437/228/171	1426/227/170	1307/219/148	999/209/144
R _{int}	6.81	8.92	4.3	5.53	4.9	6.23	4.42
No. of parameters/restraints/constraints	17/0/2						
Final R indices [I > 3σ(I)] R _F /wR _F	0.0630/0.0804	0.0619/0.0616	0.0400/0.0492	0.0598/0.0726	0.0631/0.0725	0.0473/0.0626	0.0452/0.0530
R indices (all data) R _F /wR _F	0.0699/0.0818	0.0943/0.0675	0.0507/0.0519	0.0713/0.0748	0.0725/0.0739	0.0609/0.0641	0.0609/0.0556

Largest diff. peak /hole ($e / \text{\AA}^3$)	0.91/0.87						
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N of the run	S6073						
Crystal system	cubic						
Space group	$Ia\bar{3}d$						
Z	8						
P, GPa	85.6(1)	88.62(84)	1.4	2.58(16)	3.7(5)	5.0(5)	6.19(3)
a (Å)	10.5875(10)	10.5706(10)	11.6788(2)	11.6570(2)	11.6347(2)	11.6001(1)	11.5762(1)
V (Å ³)	1186.8(2)	1181.1(4)	1592.92(5)	1584.02(5)	1574.95(5)	1560.94(2)	1551.31(2)
FeO ₈ , V ₀ , Å ³	14.7310	14.5706	20.9802	20.7998	20.6589	20.3712	20.1944
(Fe,Si)O ₆ , V ₀ , Å ³	7.4276	7.4139	10.3646	10.3150	10.2443	10.2285	10.1063
SiO ₄ , V ₀ , Å ³	1.9545	1.9576	2.2139	2.1942	2.1985	2.1842	2.1906
$F(000)$	2122	2122	2122	2122	2122	2122	2122
Theta range for data collection(°)	2.75/20.73	2.76/20.76	2.49/20.92	2.5/20.64	2.5/20.68	2.51/20.74	2.52/20.73
Index ranges	-13 < h < 16	-12 < h < 16	-13 < h < 5	-18 < h < 15	-16 < h < 16	-10 < h < 14	-9 < h < 13
	-17 < k < 13	-17 < k < 13	-18 < k < 14	-14 < k < 9	-7 < k < 14	-16 < k < 16	-16 < k < 16
	-13 < l < 11	-13 < l < 11	-16 < l < 16	-16 < l < 16	-14 < l < 18	-16 < l < 18	-16 < l < 18
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	1310/215/136	1259/217/87	1267/282/167	2030/295/218	1821/295/180	2130/290/223	2118/290/221
R_{int}	7.27	11.89	2.83	4.23	4.24	3.94	4.59
No. of parameters/restraints/constraints	17/0/2						
Final R indices [$I > 3\sigma(I)$] R_F/wR_F	0.0555/0.0586	0.0616/0.0630	0.0308/0.0398	0.0261/0.0345	0.0290/0.0365	0.0310/0.0399	0.0351/0.0424
R indices (all data) R_F/wR_F	0.0737/0.0617	0.1399/0.0727	0.0535/0.0430	0.0352/0.0365	0.0545/0.0434	0.0373/0.0423	0.0411/0.0442

Largest diff. peak /hole ($e / \text{\AA}^3$)	0.91/0.87						
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N of the run	S6073						
Crystal system	cubic						
Space group	$Ia\bar{3}d$						
Z	8						
P, GPa	7.45(3)	8.87(5)	10.23(5)	15.24(12)	19.99(11)	25.04(10)	31.5(16)
a (Å)	11.5513(1)	11.523(1)	11.5013(2)	11.4073(2)	11.3309(2)	11.2569(3)	11.1737(3)
V (Å ³)	1541.32(2)	1530.18(2)	1521.39(5)	1484.39(5)	1454.77(4)	1426.45(7)	1395.05(6)
FeO ₈ , V ₀ , Å ³	20.0193	19.8425	19.6693	19.0159	18.5027	18.0082	17.5111
(Fe,Si)O ₆ , V ₀ , Å ³	10,0797	9.9496	9.9150	9.7056	9.5548	9.4246	9.2460
SiO ₄ , V ₀ , Å ³	1.9545	2.1164	2.1609	2.1404	2.1174	2.0946	2.0633
$F(000)$	2122						
Theta range for data collection(°)	2.75/20.73	2.53/20.89	2.53/20.93	2.55/20.83	2.57/20.74	2.59/20.53	2.61/20.75
Index ranges	-13 < h < 16	-13 < h < 9	-9 < h < 13	-16 < h < 16	-7 < h < 12	-16 < h < 16	-16 < h < 16
	-17 < k < 13	-16 < k < 16	-16 < k < 18	-7 < k < 12	-17 < k < 18	-17 < k < 15	-18 < k < 15
	-13 < l < 11	-16 < l < 18	-16 < l < 16	-18 < l < 16	-16 < l < 17	-7 < l < 12	-7 < l < 12
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	1310/215/136	2103/286/236	2085/286/232	1732/274/218	1963/276/214	1694/265/200	1654/260/188
R_{int}	7.27	6.22	4.16	3.52	5.3	3.0	3.04
No. of parameters/restraints/constraints	17/0/2						
Final R indices	0.0555/0.0586	0.0286/0.0384	0.0288/0.0364	0.0273/0.0363	0.0301/0.0301	0.0394/0.0490	0.0387/0.0468

$[I > 3\sigma(I)]R_F/wR_F$							
R indices (all data) R_F/wR_F	0.0737/0.0617	0.0334/0.0397	0.0340/0.0379	0.0348/0.0387	0.0375/0.0375	0.0491/0.0517	0.0503/0.0491
Largest diff. peak /hole ($e/\text{\AA}^3$)	0.91/0.87						

Table S 2 Results of the crystal structure refinement based on single-crystal X-ray diffraction data for skiagite-majorite garnets with the composition Ski₆₉Maj₃₁ (S6176 run)

N of the run	S6176						
Crystal system	cubic						
Space group	$ Ia\bar{3}d $						
Z	8						
P, GPa	0.3(5)	1.03(5)	2.9(5)	4.89(5)	6.94(5)	9.86(5)	14.8(5)
a (Å)	11.7094(3)	11.6945(3)	11.6530(2)	11.6100(2)	11.5679(3)	11.5120(2)	11.4363(2)
V (Å ³)	1605.48(12)	1599.36(12)	1582.39(8)	1564.94(8)	1547.97(12)	1525.64(8)	1495.74(8)
FeO ₈ , V ₀ , Å ³	21.2155	21.1308	20.772	20.4502	20.1509	19.7359	19.1866
(Fe,Si)O ₆ , V ₀ , Å ³	10.3431	10.3179	10.2325	10.1364	10.0507	9.9419	9.7845
SiO ₄ , V ₀ , Å ³	2.2107	1.6348	2.1963	2.1886	2.1765	2.164	2.1487
F(000)	1152	1152	1152	3242	3243	3241	3241
Theta range for data collection(°)	2.658/17.585	1.742/17.821	1.748/17.795	1.755/17.679	1.761/17.745	1.770/ 17.834	1.782/17.703
Index ranges	-18 < h < 12	-20 < h < 20	-18 < h < 15	-19 < h < 20	-18 < h < 15	-19 < h < 10	-19 < h < 19
	-18 < k < 18	-15 < k < 18	-20 < k < 20	-15 < k < 19	-19 < k < 19	-18 < k < 15	-15 < k < 17
	-17 < l < 13	-15 < l < 19	-19 < l < 15	-15 < l < 18	-19 < l < 15	-15 < l < 18	-15 < l < 18
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	4001/415/304	4632/475/360	4575/472/356	4525/462/374	4464/460/348	4414/455/358	4295/449/344
R _{int}	0.0436	0.0452	0.0371	0.0333	0.0399	0.0319	0.0434
No.of parameters/restraints	19/0						

Final R indices $[I > 3\sigma(I)] R_F / wR_F$	0.0407/0.1023	0.0364/0.0914	0.0365/0.0932	0.0332/0.0847	0.0341/0.0898	0.0320/0.0786	0.0296/0.0799
R indices (all data) R_F / wR_F	0.0616/0.1273	0.0516/0.1050	0.0487/0.1098	0.0410/0.0928	0.0426/0.098 2	0.0419/0.0878	0.0443/0.0888
Largest diff. peak /hole ($e / \text{\AA}^3$)	-1.291/0.261	-1.238/0.227	-1.262/0.257	-1.191/0.262	-1.234/0.237	-0.999/0.234	-0.657/0.175

N of the run	S6176						
Crystal system	cubic						
Space group	$Ia\bar{3}d$						
Z	8						
P, GPa	18.39(5)	23.58(17)	28.38(5)	33.17(8)	38.48(16)	42.85(5)	46.73(5)
a (Å)	11.3653(2)	11.2905(2)	11.2250(3)	11.1624(4)	11.1005(4)	11.0511(4)	11.0102(4)
V (Å ³)	1468.06(8)	1439.26(8)	1414.36(11)	1390.83(15)	1367.82(15)	1349.64(15)	1334.71(15)
FeO ₈ , V ₀ , Å ³	18.738	18.253	17.8229	17.4541	17.0841	16.8064	16.6071
(Fe,Si)O ₆ , V ₀ , Å ³	9.6551	9.4798	9.3459	9.2228	9.1037	8.9975	8.9082
SiO ₄ , V ₀ , Å ³	2.1197	2.101	2.0827	2.0603	2.039	2.0264	2.0142
F(000)	3241	3242	3242	3239	3240	3243	3242
Theta range for data collection(°)	1.793/17.87	1.805/17.613	1.815/17.70	1.825/17.622	1.835/17.723	1.844/17.805	1.851/17.805
Index ranges	-19 < h < 19	-15 < h < 18	-17 < h < 15	-17 < h < 14	-17 < h < 14	-17 < h < 14	-18 < h < 18
	-17 < k < 15	-19 < k < 19	-19 < k < 19	-18 < k < 19	-18 < k < 18	-17 < k < 14	-17 < k < 14
	-15 < l < 18	-15 < l < 17	-18 < l < 14	-18 < l < 14	-18 < l < 14	-18 < l < 18	-14 < l < 17
No. of measured, independent, and observed [I > 3σ(I)] reflections	4187/438/345	4090/433/337	3965/425/305	3901/408/294	3822/401/281	3798/401/313	3771/396/296
R _{int}	0.0345	0.0366	0.0409	0.0443	0.0445	0.0361	0.0399
No. of parameters/restraints	19/0						
Final R indices [I > 3σ(I)] R _F /wR _F	0.0280/0.0702	0.0276/0.0681	0.0340/0.0896	0.0347/0.0830	0.0391/0.1034	0.0364/0.0859	0.0386/0.0929
R indices (all data) R _F /wR _F	0.0381/0.0841	0.0384/0.0790	0.0515/0.1054	0.0528/0.1018	0.0391/0.1034	0.0492/0.0964	0.0525/0.1042

Largest diff. peak /hole (e / Å ³)	-0.719/0.187	-0.696/ 0.186	-0.961/0.201	-0.766/0.206	-1.188/0.226	-1.231/0.289	-1.329/0.273
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N of the run	S6176							
Crystal system	cubic							
Space group	$Ia\bar{3}d$							
Z	8							
P, GPa	49.6(12)	52.0(5)	54.04(3)	55.17(5)	56.0(5)	56.97(7)	58.13(9)	60.16(9)
a (Å)	10.9774(5)	10.9448(5)	10.8932(6)	10.8801(5)	10.8559(6)	10.8453(5)	10.8159(6)	10.7828(8)
V (Å ³)	1322.81(18)	1311.06(18)	1292.6(2)	1287.95(18)	1279.4(2)	1275.63(18)	1265.3(2)	1253.7(3)
FeO ₈ , V ₀ , Å ³	16.4316	16.3077	16.102	16.0653	15.982	15.942	15.8382	15.7221
(Fe,Si)O ₆ , V ₀ , Å ³	8.8456	8.7276	8.4812	8.3721	8.2449	8.1895	8.0308	7.8845
SiO ₄ , V ₀ , Å ³	2.0019	1.9936	1.9857	1.9947	1.9944	1.9886	1.9865	1.9817
F(000)	3241	3240	3238	3234	3235	3235	3235	3235
Theta range for data collection(°)	1.856/17.757	1.862/17.638	1.870/17.724	1.873/17.746	1.877/17.432	1.879/17.450	1.884/17.499	1.890/17.554
Index ranges	-18 < h < 14	-18 < h < 18	-16 < h < 14	-16 < h < 14	-18 < h < 18	-14 < h < 16	-13 < h < 16	-13 < h < 16
	-16 < k < 14	-14 < k < 16	-18 < k < 18	-18 < k < 18	-14 < k < 16	-14 < k < 17	-14 < k < 18	-14 < k < 17
	-18 < l < 18	-14 < l < 17	-18 < l < 14	-18 < l < 14	-14 < l < 17	-18 < l < 18	-18 < l < 18	-18 < l < 17
No. of measured, independent, and observed [I > 3σ(I)] reflections	3718/394/293	3687/391/271	3572/386/241	3580/385/276	3522/383/259	3594/379/291	3551/377/281	3475/373/272
R _{int}	0.0385	0.0579	0.0694	0.0528	0.0680	0.0372	0.0470	0.0546
No. of parameters/restraints	19/0							
Final R indices [I > 3σ(I)] R _F /wR _F	0.0375/0.0932	0.0387/0.1001	0.0533/0.1391	0.0372/0.0943	0.0485/0.1215	0.0395/0.1052	0.0545/0.1152	0.0615/0.1243

R indices (all data) R_F/wR_F	0.0516/0.1023	0.0594/0.1131	0.0792/0.1635	0.0565/0.1075	0.074/0.1384	0.0512/0.1140	-1.307/0.335	-1.173/0.313
Largest diff. peak /hole ($e / \text{\AA}^3$)	-1.196/0.258	-1.091/0.214	-0.998/0.288	-0.893/0.259	-0.809/0.300	-1.635/0.361	-0.657/0.175	-0.657/0.175

Table S 3 Results of the crystal structure refinement based on single-crystal X-ray diffraction data for skiagite-majorite garnets with the composition Ski₅₄Maj₄₆ (S6177 run)

N of the run	S6177						
Crystal system	cubic						
Space group	$ Ia\bar{3}d $						
Z	8						
P, GPa	0.3(5)	1.03(5)	2.9(5)	4.89(5)	6.94(5)	9.86(5)	14.8(5)
a (Å)	11.6958(3)	11.6768(3)	11.6360(3)	11.5945(3)	11.5527(3)	11.4984(3)	11.4199(3)
V (Å ³)	1599.89(12)	1592.10(12)	1575.47(12)	1558.68(12)	1541.88(12)	1520.24(12)	1489.32(12)
FeO ₈ , V ₀ , Å ³	21.2752	21.0777	20.7748	20.4598	20.1553	19.7663	19.1954
(Fe,Si)O ₆ , V ₀ , Å ³	10.2376	10.1766	10.0838	9.9915	9.9303	9.8106	9.6539
SiO ₄ , V ₀ , Å ³	2.1944	2.2066	2.1957	2.1879	2.1714	2.1604	2.143
F(000)	3223	3219	3220	3220	3220	3221	3221
Theta range for data collection(°)	1.742/17.849	1.745 /17.758	1.751/ 17.638	1.757/ 17.703	1.764/ 17.769	1.772/17.793	1.784/17.472
Index ranges	-19 < h < 21	-22 < h < 21	-22 < h < 21	-22 < h < 21	-22 < h < 21	-21 < h < 21	-21 < h < 20
	-13 < k < 15	-22 < k < 21	-22 < k < 14	-22 < k < 14	-22 < k < 21	-22 < k < 21	-21 < k < 21
	-19 < l < 20	-15 < l < 16	-14 < l < 16	-14 < l < 16	-14 < l < 16	-14 < l < 16	-14 < l < 16
No. of measured, independent, and observed [I > 3σ (I)] reflections	4042/518/304	4592/539/339	4568/530/373	4482/523/373	4422/510/370	4343/503/353	4259/495/317
R _{int}	0.0528	0.0966	0.0538	0.0567	0.0528	0.0558	0.0900
No.of parameters/restraints	19/0						

Final R indices [$I > 3\sigma(I)$] R_F/wR_F	0.0407/0.0805	0.0394/0.0994	0.0340/0.0879	0.0353/0.0882	0.0367/0.0838	0.0320/0.0862	0.0392/0.0946
R indices (all data) R_F/wR_F	0.0742/0.0805	0.0628/0.1191	0.0501/0.1010	0.0513/0.1031	0.0527/0.0913	0.0560/0.1046	0.0703/0.1210
Largest diff. peak /hole ($e / \text{\AA}^3$)	-0.593/0.188	-1.235/0.256	-1.225/ 0.219	-0.958/0.209	-1.031/0.216	-0.843/0.195	-1.089/0.209

N of the run	S6177						
Crystal system							
Space group							
Z							
P, GPa	18.39(5)	23.58(17)	28.38(5)	33.17(8)	38.48(16)	42.85(5)	46.73(5)
a (Å)	11.3545(3)	11.2812(4)	11.2123(4)	11.1518(3)	11.0905(4)	11.0415(5)	11.0014(4)
V (Å ³)	1463.88(12)	1435.71(9)	1409.56(9)	1386.87(11)	1364.12(15)	1346.12(18)	1331.51(8)
FeO ₈ , V ₀ , Å ³	18.7565	18.2748	17.8608	17.4433	17.0804	16.824	16.6238
(Fe,Si)O ₆ , V ₀ , Å ³	9.4949	9.3549	9.2176	9.085	8.9661	8.8691	8.7892
SiO ₄ , V ₀ , Å ³	2.1282	2.1043	2.0781	2.0716	2.0492	2.036	2.016
F(000)	3221	3221	3221	5110	5110	5110	2102
Theta range for data collection(°)	1.794/17.576	1.81/17.69	1.8/17.63	1.827/17.773	1.837/17.536	1.845/17.582	1.81/17.2
Index ranges	-14 < h < 16	-16 < h < 14	-16 < h < 14	-15 < h < 13	-15 < h < 13	-13 < h < 14	-13 < h < 14
	-21 < k < 20	-21 < k < 20	-21 < k < 20	-20 < k < 20	-20 < k < 19	-19 < k < 20	-19 < k < 20
	-21 < l < 20	-21 < l < 20	-21 < l < 20	-21 < l < 19	-15 < l < 13	-19 < l < 20	-19 < l < 20
No. of measured, independent, and observed [I > 3σ(I)] reflections	4197/485/344	4123/482/282	4026/469/267	3971/458/ 347	3887/452/346	3810/45/341	3750/432/301
R _{int}	0.0528	0.0966	0.0538	0.0518	0.0491	0.0483	0.0435
No. of parameters/restraints	19/0						
Final R indices [I > 3σ(I)] R _F /wR _F	1.020	1.027	1.081	0.0397/0.0903	0.0398/0.0887	0.0535/0.1021	0.0376/0.0481
R indices (all data) R _F /wR _F	0.0407/0.0805	0.0394/0.0994	0.0340/0.0879	0.0544/0.1039	0.0573/0.0985	0.0399/0.0920	0.0544/0.0505
Largest diff. peak /hole (e / Å ³)	0.0742/0.0805	0.0628/0.1191	0.0501/0.1010	-1.412/0.338	-1.286/0.366	-1.354/0.340	-1.354/0.340

N of the run	S6177							
Crystal system	cubic							
Space group	$Ia\bar{3}d$							
Z	8							
P, GPa	49.6(12)	52.0(5)	54.04(3)	55.17(5)	56.0(5)	56.97(7)	58.13(9)	60.16(9)
a (Å)	10.9694(5)	10.9392(4)	10.8993(4)	10.8835(4)	10.8643(4)	10.8391(4)	10.8129(4)	10.7843(4)
V (Å ³)	1319.92(10)	1309.05(8)	1294.78(8)	1289.16(8)	1282.35(8)	1273.44(8)	1264.23(8)	1254.23(8)
FeO ₈ , V ₀ , Å ³	16.4411	16.2985	16.1649	16.1077	16.0459	15.9789	15.8577	15.7631
(Fe,Si)O ₆ , V ₀ , Å ³	8.7103	8.6057	8.4300	8.3347	8.2123	8.0683	7.9501	7.8373
SiO ₄ , V ₀ , Å ³	2.0124	2.01	2.0045	2.0057	2.0037	2.0067	2.0033	2.0022
F(000)	5110	5110	5110	2102	2101	2102	2097	2099
Theta range for data collection(°)	1.827/17.773	1.837/17.536	1.845/17.582	1.81/17.2	1.81/17.2	1.81/17.2	1.88/17.71	1.88/17.58
Index ranges	-15 < h < 13	-15 < h < 13	-13 < h < 14	-13 < h < 14	-13 < h < 14	-13 < h < 14	-19 < h < 20	-19 < h < 20
	-20 < k < 20	-20 < k < 19	-19 < k < 20	-19 < k < 20	-19 < k < 20	-19 < k < 20	-19 < k < 20	-19 < k < 20
	-21 < l < 19	-15 < l < 13	-19 < l < 20	-19 < l < 20	-20 < l < 20	-20 < l < 20	-12 < l < 14	-12 < l < 14
No. of measured, independent, and observed [I > 3σ (I)] reflections	3971/458/347	3887/452/346	3810/45/341	3750/432/301	3731/434/296	3698/431/292	3545/417/275	3516/413/284
R _{int}	0.0518	0.0491	0.0483	0.0435	0.0575	0.0568	0.0656	0.0664
No. of parameters/restraints	18/0/2							
Final R indices	2.52	2.69	1.79	1.87	1.42	2.02	2.12	1.79

$[I > 3\sigma(I)]R_F/wR_F$								
R indices (all data) R_F/wR_F	0.0424/0.0710	0.0475/0.0725	0.0353/0.0472	0.0377/0.0559	0.0344/0.0426	0.0398/0.0579	0.0462/0.0607	0.0400/0.0496
Largest diff. peak /hole (e / Å ³)	0.0597/0.0730	0.0648/0.0741	0.0517/0.0489	0.0571/0.0592	0.0564/0.0472	0.0666/0.0614	0.0674/0.0632	0.0564/0.0521

Table S 4 Results of the crystal structure refinement based on single-crystal X-ray diffraction data for skiagite-majorite garnets with the composition $\text{Ski}_{24}\text{Maj}_{76}$ (S6160 run)

N of the run	S6160						
Crystal system							
Space group							
Z							
P, GPa	0.3(5)	1.03(5)	2.9(5)	4.89(5)	6.94(5)	9.86(5)	14.8(5)
a (Å)	11.6685(3)	11.6556(3)	11.6149(2)	11.5736(2)	11.5321(3)	11.4785(2)	11.4079(2)
V (Å ³)	1588.71(12)	1583.45(12)	1566.92(8)	1550.26(8)	1533.65(12)	1512.36(8)	1484.63(8)
FeO ₈ , V ₀ , Å ³	21.205	21.125	20.817	20.504	20.181	19.7797	19.2899
(Fe,Si)O ₆ , V ₀ , Å ³	9.97	9.939	9.857	9.787	9.6776	9.5734	9.4445
SiO ₄ , V ₀ , Å ³	2.208	2.204	2.194	2.182	2.1791	2.1687	2.1445
$F(000)$	1152	1152	1152	1152	1152	1152	1152
Theta range for data collection(°)	1.746/17.771	1.748/17.852	1.754/17.856	1.760/17.798	1.767/17.424	1.775/17.508	1.786/17.620
Index ranges	-22 < h < 21	-20 < h < 20	-18 < h < 15	-20 < h < 20	-18 < h < 15	-20 < h < 20	-20 < h < 20
	-24 < k < 21	-21 < k < 21	-21 < k < 21	-21 < k < 21	-20 < k < 20	-21 < k < 22	-21 < k < 21
	-12 < l < 17	-18 < l < 15	-20 < l < 20	-18 < l < 15	-21 < l < 21	-15 < l < 18	-17 < l < 14
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	4069/530/345	4627/529/369	4551/519/386	4502/516/371	4467/515/380	4377/510/387	4290/503/373
R_{int}	0.0441	0.0587	0.0382	0.0504	0.0460	0.0398	0.0641

No. of parameters/restraints	21/0	21/0	19/0				
Final R indices $[I > 3\sigma(I)] R_F / wR_F$	0.0338/0.0875	0.0348/0.0880	0.0286/0.0695	0.0434/0.0689	0.0327/0.0800	0.0299/0.0706	0.0333/0.0809
R indices (all data) R_F / wR_F	0.0593/0.1057	0.0523/0.1055	0.0404/0.0821	0.0434/0.0801	0.0479/0.1003	0.0412/0.0819	0.0454/0.0930
Largest diff. peak /hole ($e / \text{\AA}^3$)	-0.719/0.203	-1.087/0.261	-0.900/0.199	-0.677/0.186	-1.120/ 0.220	-0.837/0.223	-1.090/0.266

N of the run	S6160						
Crystal system							
Space group							
Z							
P, GPa	18.39(5)	23.58(17)	28.38(5)	33.17(8)	38.48(16)	42.85(5)	46.73(5)
<i>a</i> (Å)	11.3380(2)	11.2614(2)	11.2040(3)	11.1389(3)	11.0770(3)	11.0230(4)	10.9803(4)
<i>V</i> (Å ³)	1457.50(8)	1428.16(8)	1406.43(11)	1382.06(11)	1359.15(11)	1339.37(15)	1323.86(14)
FeO ₈ , V ₀ , Å ³	18.8227	18.3134	17.9151	17.5099	17.1523	16.8364	16.6161
(Fe,Si)O ₆ , V ₀ , Å ³	9.291	9.1163	9.0334	8,8795	8.7735	8.6456	8.5579
SiO ₄ , V ₀ , Å ³	2.1275	2.1118	2.0924	2.0784	2.0513	2.0359	2.0242
<i>F</i> (000)	1152	1152	1152	1152	1152	1152	1152
Theta range for data collection(°)	1.797/17.732	1.809/17.726	1.819/17.787	1.829/17.794	1.839/17.830	1.848/ 17.647	1.856/17.718
Index ranges	-20 < h <20,	-14< h <17,	-21< h <21,	-21 < h < 21,	-21 < h < 21,	-20 < h < 20,	-20 < h < 19,
	-21< k <21,	-20< k <20,	-19< k <20,	-20 < k < 20,	-20 < k < 20,	-21 < k < 21,	-21 < k < 21,
	-17< l <14	-21< l <21	-17< l <14	-18< l <14	-18< l <14	-14< l <17	-14< l <17
No. of measured, independent, and observed [<i>I</i> > 3σ(<i>I</i>)] reflections	4196/495/372	4116/484/377	4062/478/347	3987/476/ 354	3906/470/ 351	3832/461/341	3738/451/329
<i>R</i> _{int}	0.0521	0.0403	0.0563	0.0513	0.0532	0.0481	0.0449
No.of parameters/restraints			19/0	19/0			
Final R indices [<i>I</i> >3σ(<i>I</i>)] <i>R</i> _F / <i>wR</i> _F	1.107	1.103	1.115	1.101	1.160	1.014	1.063
R indices (all data) <i>R</i> _F / <i>wR</i> _F	0.0352/0.0825	0.0378/0.0959	0.0383/0.0871	0.0380/0.0881	0.0310/0.0716	0.0291/0.0725	0.0351/0.0865

Largest diff. peak /hole ($e / \text{\AA}^3$)	0.0473/0.0976	0.0470/0.1059	0.0524/0.1012	0.0491/0.1044	0.0450/0.0884	0.0459/0.0809	0.0513/0.1000
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N of the run	S6160							
Crystal system	cubic							
Space group	$ Ia\bar{3}d $							
Z	8							
P, GPa	49.6(12)	52.0(5)	54.04(3)	55.17(5)	56.0(5)	56.97(7)	58.13(9)	60.16(9)
a (Å)	10.9497(5)	10.9211(5)	10.8804(5)	10.8640(5)	10.8520(5)	10.8298(5)	10.8070(5)	10.7831(5)
V (Å ³)	1312.82(18)	1302.56(18)	1288.06(18)	1282.24(18)	1278.00(18)	1270.17(18)	1262.16(18)	1253.81(17)
FeO ₈ , V ₀ , Å ³	16.4451	16.3339	16.1645	16.1176	16.0563	15.9738	15.9662	15.8018
(Fe,Si)O ₆ , V ₀ , Å ³	8.5047	8.4223	8.234	8.1582	8.0879	7.9683	7.8638	7.7668
SiO ₄ , V ₀ , Å ³	2.0135	2.0021	1.9995	1.9936	1.9979	1.9979	1.9904	1.9905
$F(000)$	1152	1152	1152	1152	1152	1152	1152	1152
Theta range for data collection(°)	1.861/17.734	1.866/17.782	1.873/17.675	1.875/17.703	1.878/17.581	1.881/17.619	1.885/17.657	1.890/17.626
Index ranges	-20 < h < 19	-20 < h < 19	-19 < h < 19	-19 < h < 19	-19 < h < 19	-18 < h < 14	-21 < h < 21	-18 < h < 15
	-21 < k < 21	-21 < k < 21	-21 < k < 21	-21 < k < 21	-21 < k < 21	-21 < k < 21	-20 < k < 20	-21 < k < 21
	-14 < l < 17	-14 < l < 17	-14 < l < 17	-14 < l < 17	-14 < l < 17	-19 < l < 19	-18 < l < 14	-19 < l < 19
No. of measured, independent, and observed [$I > 3\sigma(I)$] reflections	3723/447/321	3682/444/316	3647/438/302	3620/435/302	3622/432/307	3602/433/314	3612/434/310	3592/433/309
R_{int}	0.0481	0.0443	0.0545	0.0457	0.0541	0.0558	0.0560	0.0552
No. of parameters/restraints	19/0							
Final R indices [$I > 3\sigma(I)$] R_F/wR_F	0.0397/0.0970	0.0381/0.0985	0.0371/0.0963	0.0358/0.0936	0.0348/0.0904	0.0371/0.0929	0.0414/0.1060	0.0395/0.0998
R indices (all data)	0.0566/0.1188	0.0555/0.1144	0.0547/0.1143	0.0534/0.1174	0.0515/0.1081	0.0539/0.1097	0.0596/0.1258	0.0545/0.1175

R_F/wR_F								
Largest diff. peak /hole ($e / \text{\AA}^3$)	-0.733/ 0.240	-0.673/0.223	-0.696/0.208	-0.731/0.228	-0.805/ 0.199	-0.987/ 0.221	-1.116/0.290	-1.092/ 0.302

Table S 5 Results of the fit of the P-V experimental data using the 2nd order Birch-Murnaghan equation of state.

Composition	Results of the fit with the 2 nd order Birch-Murnaghan equation of state (K' fixed at 4)			
	unit cell	(Fe,Si)O ₆	FeO ₈	SiO ₄
	V ₀ , Å ³	V ₀ , Å ³	V ₀ , Å ³	V ₀ , Å ³
	K _{0,300} , GPa	K _{0,300} , GPa	K _{0,300} , GPa	K _{0,300} , GPa
Ski _{76.6} Maj _{23.4}	High Spin	High Spin	21.35(2)	2.214(2)
	1608.1(4)	10.349(7)	101(1)	386(7)
	162.4(6)	216(2)		
	Low Spin	Low Spin		
	1435(11)	9.14(15)		
	306(18)	271(30)		
Ski ₆₉ Maj ₃₁	1606(2)	10.336(9)	21.25(4)	2.213(1)
	172(1)	232(2)	115(1)	405(3)
Ski ₅₄ Maj ₄₆	1603.91	10.335(9)	21.23	2.209(2)
	171.8(3)	233(2)	115(2)	482(9)
Ski ₂₄ Maj ₇₆	1591.8(8)	9.971(13)	21.34(3)	2.208(1)
	174(2)	227(3)	112.8(9)	483(7)
Ski ₁₀₀ (Woodland et al. 1999)	1610.8(3)	-	-	-
	169(1)			