Appendix 1. Tables of structural parameters

Table A1 Unit-cell parameters of z626-wadsleyite at different temperatures. *Standard deviations in parentheses result from Rietveld fits.*

T (K)	*a*(Å)	*b*(Å)	*c*(Å)	*V*(Å^3)
297	5.70158(8)	11.44275(16)	8.24913(12)	538.188(13)
297*	5.70032(8)	11.44070(16)	8.25282(12)	538.213(13)
343	5.70334(10)	11.44579(20)	8.25358(14)	538.788(16)
389	5.70496(10)	11.44901(20)	8.25756(14)	539.352(16)
437	5.70698(10)	11.45336(20)	8.26188(14)	540.030(16)
484	5.70934(10)	11.45695(21)	8.26654(14)	540.728(16)
532	5.71185(10)	11.46233(21)	8.27199(14)	541.576(17)
581	5.71434(11)	11.46594(21)	8.27682(14)	542.300(17)
629	5.71632(11)	11.47040(22)	8.28235(15)	543.061(18)
678	5.71885(11)	11.47449(22)	8.28653(14)	543.770(18)
728	5.72145(11)	11.47888(22)	8.29240(15)	544.610(18)
777	5.72370(11)	11.48366(22)	8.29757(15)	545.391(18)
827	5.72685(12)	11.48883(23)	8.30394(15)	546.356(18)
878	5.72956(11)	11.49445(23)	8.31005(15)	547.285(18)
929	5.73213(12)	11.49976(23)	8.31632(15)	548.196(19)
980	5.73474(12)	11.50466(23)	8.32281(15)	549.108(19)
1031	5.73699(12)	11.50964(24)	8.32892(16)	549.964(19)
1084	5.73907(12)	11.51340(24)	8.33503(16)	550.747(19)

*Lattice parameters after high-temperature diffraction

Table A2 Unit-cell parameters of z627-wadsleyite at different temperatures. *Standard deviations in parentheses result from Rietveld fits.*

T (K)	*a*(Å)	*b*(Å)	*c*(Å)	*V*(Å^3)
297	5.70297(12)	11.44477(23)	8.24998(15)	538.469(18)
297*	5.6915(7)	11.4257(14)	8.2516(8)	536.6(1)
320	5.70411(12)	11.44737(24)	8.25218(16)	538.843(19)
366	5.70616(12)	11.45068(24)	8.25611(16)	539.450(19)
413	5.70823(12)	11.45481(24)	8.26033(16)	540.116(19)
461	5.71066(12)	11.45883(24)	8.26515(17)	540.851(20)
508	5.71279(13)	11.46315(25)	8.27032(17)	541.594(20)
566	5.71523(13)	11.46836(26)	8.27558(17)	542.417(21)
605	5.71744(13)	11.47217(27)	8.27970(18)	543.077(21)
654	5.71958(13)	11.47635(25)	8.28483(17)	543.815(20)
703	5.72242(14)	11.48111(29)	8.29052(19)	544.685(23)
753	5.72479(13)	11.48593(25)	8.29583(17)	545.488(21)
802	5.72763(13)	11.49106(26)	8.30154(18)	546.379(21)
853	5.73026(14)	11.49593(27)	8.30719(18)	547.234(22)
903	5.73339(14)	11.50173(27)	8.31376(18)	548.242(22)
955	5.73596(14)	11.50643(28)	8.31947(19)	549.088(23)
1006	5.73790(15)	11.51061(30)	8.32505(20)	549.842(24)
1058	5.74067(14)	11.51626(28)	8.33129(19)	550.791(23)
1110§	5.74364(15)	11.52211(29)	8.33924(20)	551.881(24)
1163§	5.74303(37)	11.5213(40)	8.34814(48)	552.373(60)

*Lattice parameters after high-temperature diffraction up to 1163 K: sample is a mixture of wadsleyite (11%), forsterite (88%, *a*=4.7540(2), *b*=10.2127(7) Å, *c*=5.9845(4) Å, *V*=290.55(3) Å^3) and periclase (1%); *the decrease of volume is result of strong overlapping of diffraction peaks of wadsleyite and forsterite along with minor amount of wadsleyite and reflection broadening.*

§growing up in forsterite content:

1110 K – wadsleyite (91%) + forsterite (8%, *a*=4.8083(5), *b*=10.3089(14) Å, *c*=6.0377(8) Å, *V*=299.28(7) Å^3) + periclase (1%);

1163 K – wadsleyite (44%) + forsterite (55%, a=4.8026(4), b=10.3115(8) Å, c=6.0430(4) Å, V=299.26(4) Å^3) + periclase (1%)

Table A3 Unit-cell parameters of forsterite at different temperatures. Standard deviations of lattice parameters (*as result of le Bail fits*) are in the order of 0.0001 Å for a and b, 0.0002 Å for c and 0.01 Å^3 for volume.

T (K)	a(Å)	b(Å)	c(Å)	V(Å^3)
299	4.7543	10.1976	5.9813	289.99
314.6	4.7549	10.1997	5.9824	290.14
335.4	4.7556	10.2022	5.9838	290.32
356.2	4.7564	10.2049	5.9853	290.51
377	4.7572	10.2076	5.9867	290.71
397.8	4.7581	10.2107	5.9883	290.93
418.6	4.7589	10.2134	5.9898	291.13
439.4	4.7597	10.2165	5.9913	291.35
460.2	4.7605	10.2195	5.9930	291.56
481	4.7615	10.2226	5.9945	291.78
501.8	4.7624	10.2256	5.9960	292.00
522.6	4.7633	10.2288	5.9978	292.23
543.4	4.7642	10.2317	5.9993	292.45
564.2	4.7651	10.2348	6.0009	292.66
585	4.7660	10.2378	6.0025	292.88
605.8	4.7669	10.2407	6.0041	293.10
626.6	4.7679	10.2438	6.0058	293.33
647.4	4.7689	10.2469	6.0074	293.56
668.2	4.7697	10.2501	6.0090	293.78
689	4.7707	10.2530	6.0107	294.01
709.8	4.7716	10.2560	6.0122	294.22
730.6	4.7726	10.2592	6.0140	294.46
751.4	4.7736	10.2623	6.0156	294.69
772.2	4.7744	10.2656	6.0172	294.92
793	4.7755	10.2687	6.0189	295.15
813.8	4.7765	10.2719	6.0206	295.39
834.6	4.7774	10.2751	6.0223	295.63
855.4	4.7783	10.2782	6.0239	295.85
876.2	4.7793	10.2815	6.0256	296.09
897	4.7803	10.2846	6.0273	296.33
917.8	4.7813	10.2880	6.0291	296.57
938.6	4.7823	10.2913	6.0309	296.81
959.4	4.7833	10.2946	6.0325	297.05
980.2	4.7843	10.2977	6.0341	297.28
1001	4.7853	10.3011	6.0358	297.53
1021.8	4.7863	10.3043	6.0376	297.77
1042.6	4.7872	10.3074	6.0393	298.00
1063.4	4.7882	10.3106	6.0409	298.24
1084.2	4.7893	10.3139	6.0427	298.49
1105	4.7903	10.3173	6.0444	298.73
1125.8	4.7913	10.3203	6.0461	298.96
1146.6	4.7923	10.3236	6.0478	299.21
1167.4	4.7933	10.3267	6.0494	299.44
1188.2	4.7943	10.3299	6.0512	299.68
1209	4.7953	10.3330	6.0529	299.92
1229.8	4.7963	10.3364	6.0546	300.16
1250.6	4.7973	10.3396	6.0563	300.41
1271.4	4.7983	10.3426	6.0579	300.63

1292.2	4.7993	10.3459	6.0596	300.88
1313	4.8003	10.3490	6.0614	301.12

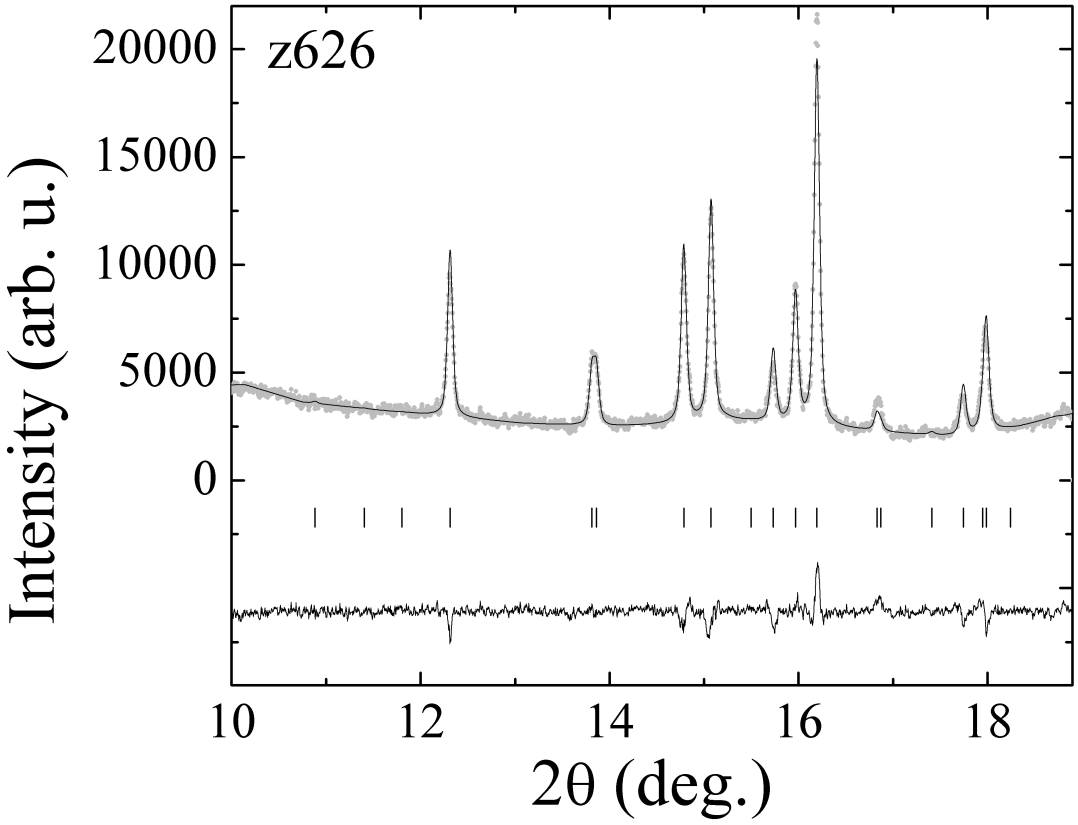
Table A4 Structural parameters of wadsleyite (for pure z626) at selected temperatures. Atoms are labeled as in reference (Jacobsen et al. 2005) and figure 1. Occupancies were fixed corresponding to the ideal stoichiometry; overall isotropic displacement factor was used for description of atomic displacement parameters.

T (K)	297	728	929	1084
Symmetry	*Imma*	*Imma*	*Imma*	*Imma*
a (Å)	5.70158(8)	5.72145(11)	5.73213(12)	5.73907(12)
b (Å)	11.44275(16)	11.47888(22)	11.49976(23)	11.51340(24)
c (Å)	8.24913(12)	8.29240(15)	8.31632(15)	8.33503(16)
V (Å^3)	538.188(13)	544.610(18)	548.196(19)	550.747(19)
	Mg1 at 4a			
x/a	0	0	0	0
y/b	0	0	0	0
z/c	0	0	0	0
	Mg2 at 4e			
x/a	0	0	0	0
y/b	¼	¼	¼	¼
z/c	0.9726(4)	0.9711(5)	0.9697(5)	0.96705(5)
	Mg3 at 8g			
x/a	¼	¼	¼	¼
y/b	0.1286(4)	0.1280(4)	0.1301(5)	0.1286(5)
z/c	¼	¼	¼	¼
	Si at 8h			
x/a	0	0	0	0
y/b	0.1187(3)	0.1196(3)	0.1188(3)	0.1203(3)
z/c	0.6175(4)	0.6175(4)	0.6163(4)	0.6168(4)
	O1 at 4e			
x/a	0	0	0	0
y/b	¼	¼	¼	¼
z/c	0.2177(9)	0.2148(9)	0.2164(9)	0.2152(9)
	O2 at 4e			
x/a	0	0	0	0
y/b	¼	¼	¼	¼
z/c	0.7179(9)	0.7195(9)	0.7146(10)	0.7154(10)
	O3 at 8h			
x/a	0	0	0	0
y/b	0.9929(4)	0.9915(4)	0.9907(4)	0.9912(4)
z/c	0.2548(9)	0.2561(9)	0.2538(10)	0.2551(10)
	O4 at 16j			
x/a	0.2624(5)	0.2631(5)	0.2639(5)	0.2657(5)
y/b	0.1227(12)	0.1226(14)	0.1235(13)	0.1256(15)
z/c	0.9945(4)	0.9942(4)	0.9939(5)	0.9939(4)
B_{ov} (Å^2)	0.12(4)	0.23(3)	0.41(4)	0.39(4)
Number of "independent" reflections*	396	401	402	405
Effective number (account for resolution) of reflections with *p*=0.5*	183	173	178	170
R_{Bragg} (%), R_F (%), $\chi 2$	4.7, 6, 9.9	4.8, 6.1, 10.4	4.9, 6.4, 10.8	4.7, 6, 10.2

*– see FullProf manual for exact meaning of these parameters.

Appendix 2. Graphical representations of results of Rietveld refinements or Le bail fits for selected diffraction patterns.

Figure A.2.1. Results of Rietveld refinements of wadsleyite (orthorhombic, space group *Imma*) samples. Experimental data (grey circles) and the calculated profile (solid line through the circles) are presented together with the calculated Bragg positions (vertical ticks) and the difference curve (solid line below). z626 is pure sample (a), whereas traces of forsterite (orthorhombic, space group *Pbnm*, displayed by black arrows) and periclase (cubic, space group $Fm\bar{3}m$, grey arrow) are visible in the diffraction pattern of z627 (b). Upper, middle and lower rows of vertical ticks in diffraction pattern of z627 correspond to calculated Bragg positions of wadsleyite, forsterite and periclase, respectively.



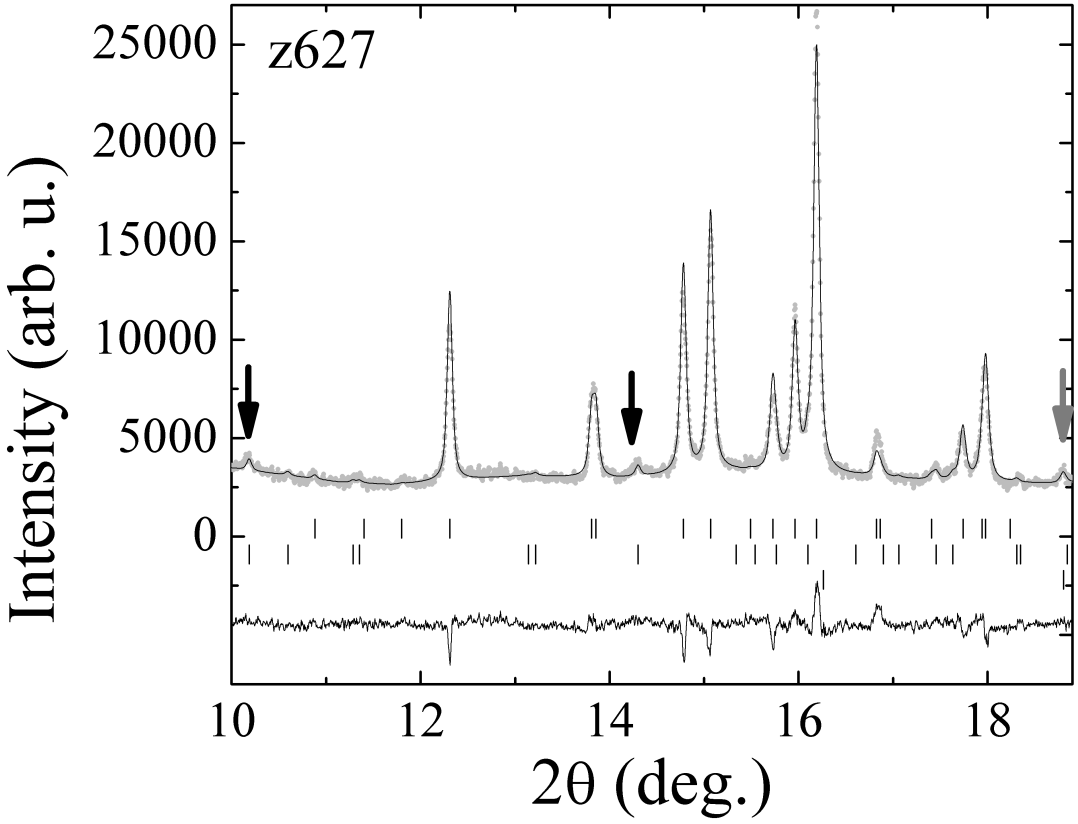
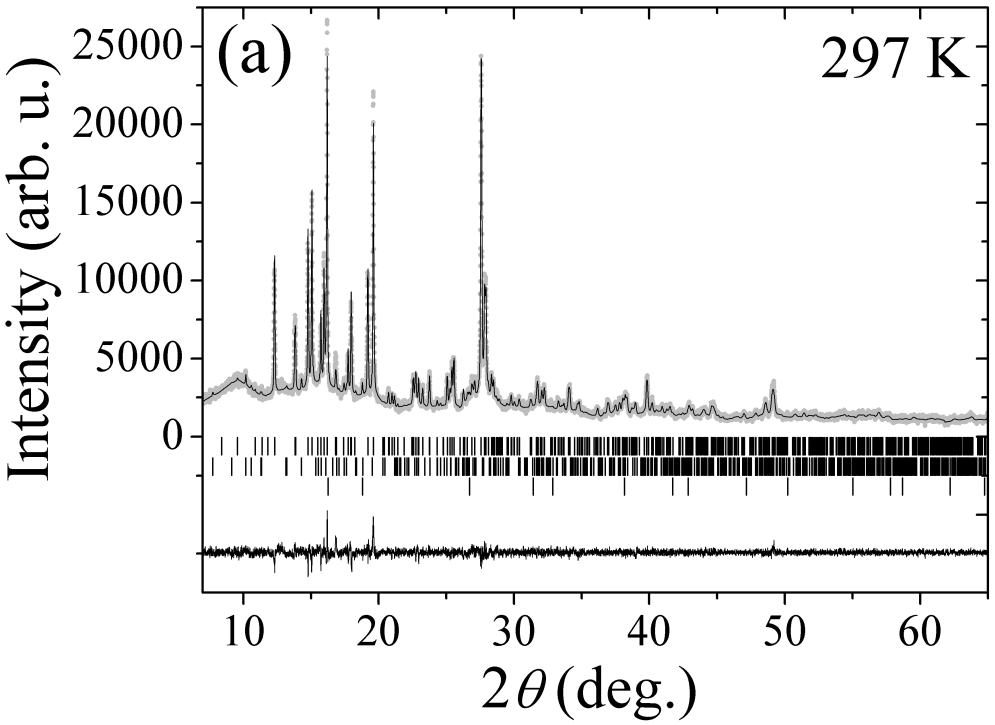
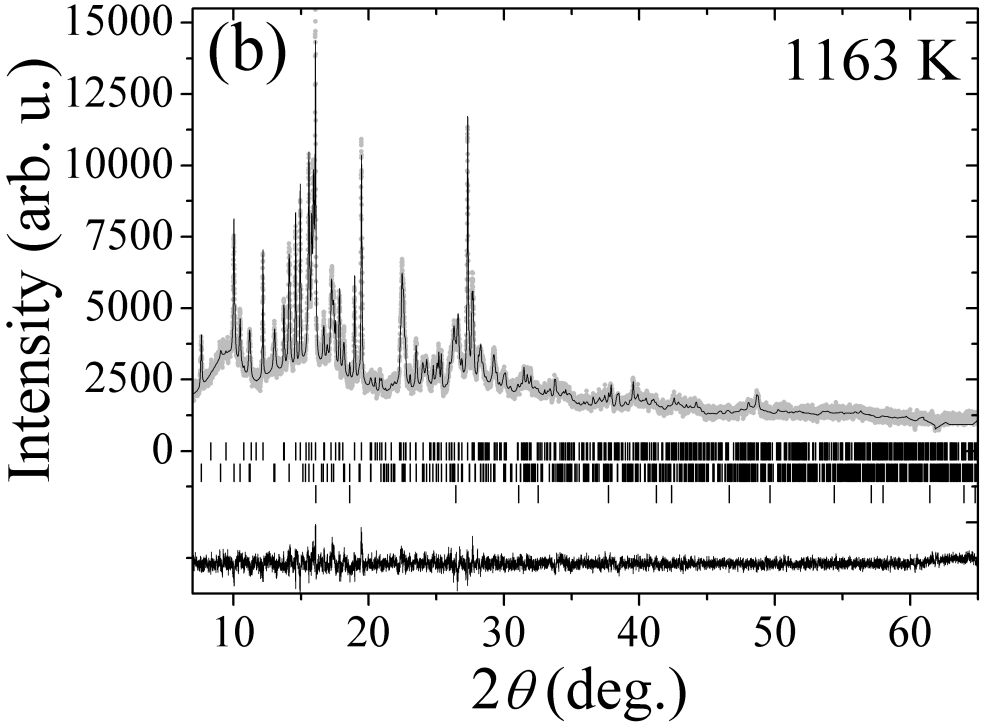
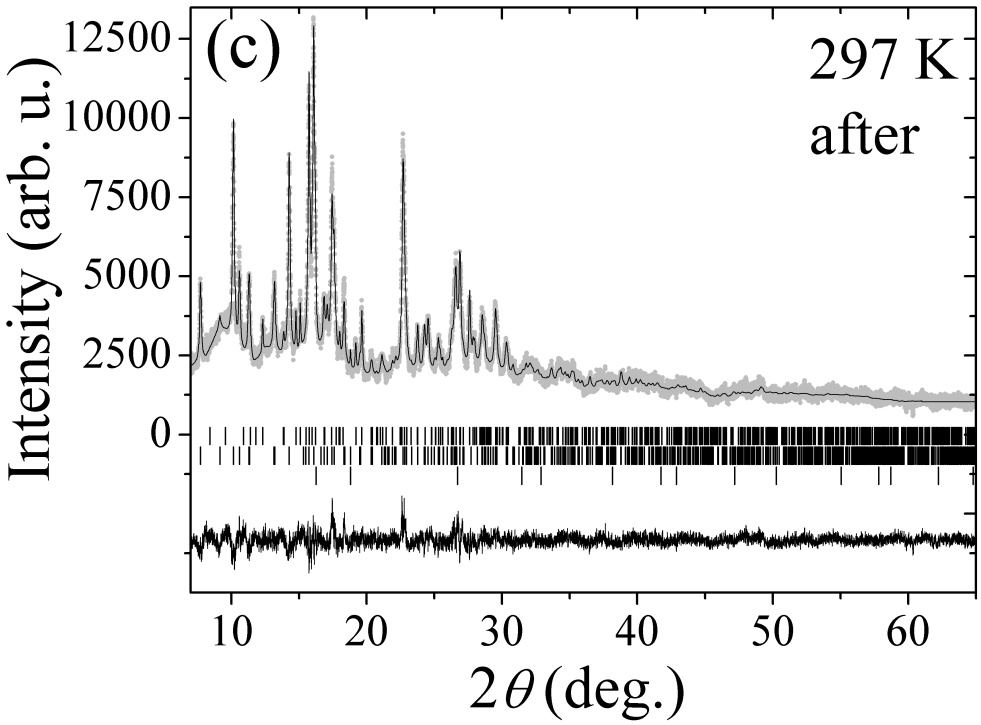
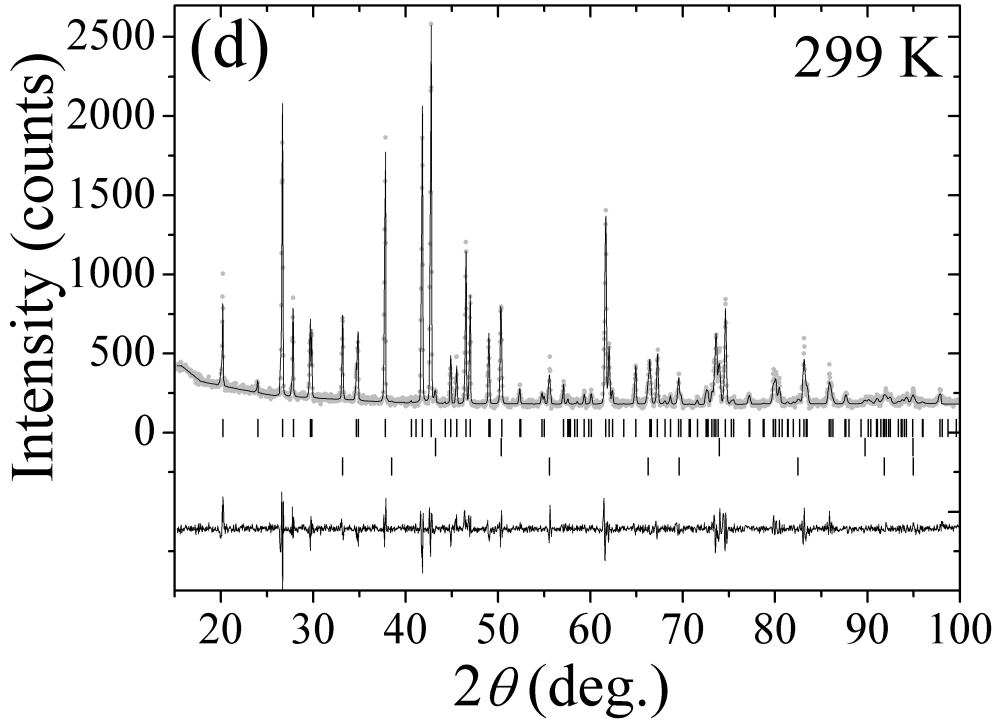


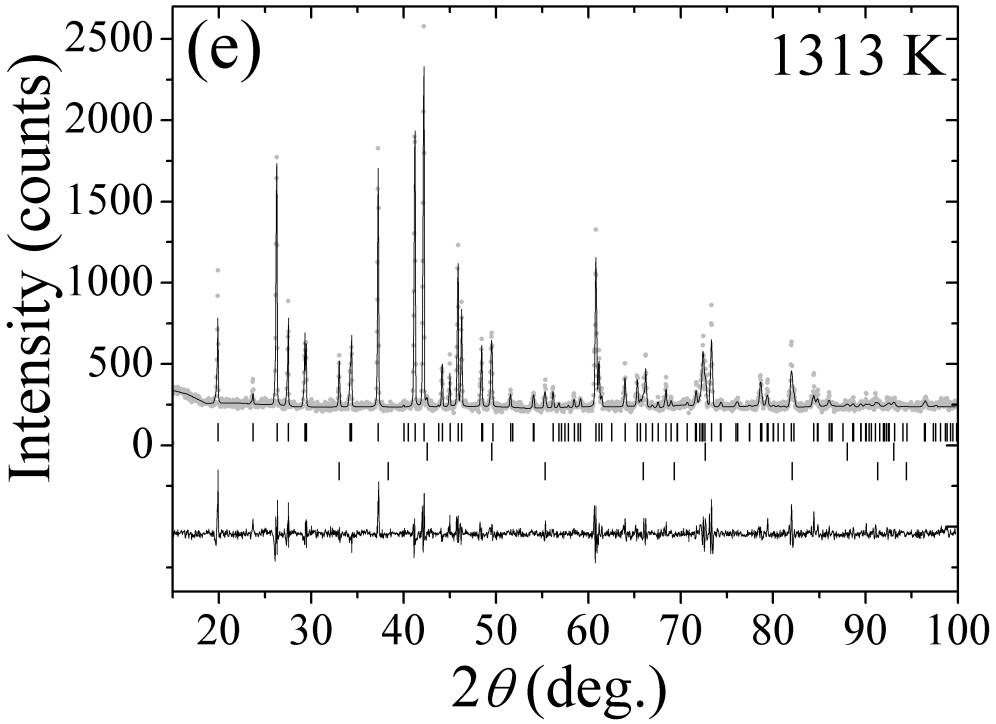
Figure A.2.2. (a–c) – results of Rietveld refinements of z627 at room temperature (94% wadsleyite, 1% periclase and 5% forsterite), 1163 K (44% wadsleyite, 1% periclase and 55% forsterite) and at room temperature after high temperature diffraction (11% wadsleyite, 1% periclase and 88% forsterite). (d and e) – an example of Le Bail fits for forsterite at lowest and highest experimental temperatures – upper, middle and lower rows of calculated Bragg maxima belong to forsterire, MgO and Si, respectively. Symbols as in figure A.2.1.


(a)
297 K
Intensity (arb. u.)
25000
20000
15000
10000
5000
0
10
20
30
40
50
60
2θ (deg.)


(b)
1163 K
Intensity (arb. u.)
15000
12500
10000
7500
5000
2500
0
10
20
30
40
50
60
2θ (deg.)

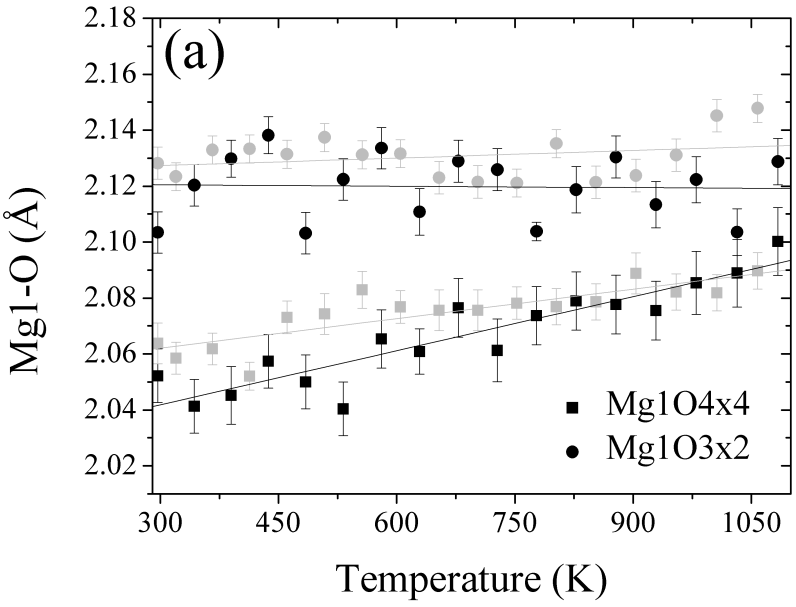

(c)
297 K
after
Intensity (arb. u.)
12500
10000
7500
5000
2500
0
10
20
30
40
50
60
2θ (deg.)


(d)
299 K
Intensity (counts)
2500
2000
1500
1000
500
0
20
30
40
50
60
70
80
90
100
2θ (deg.)

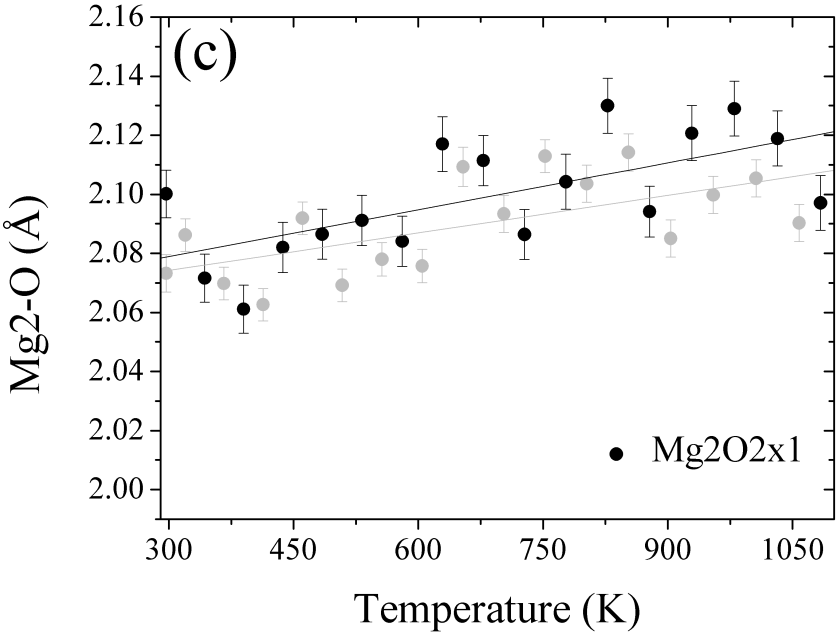


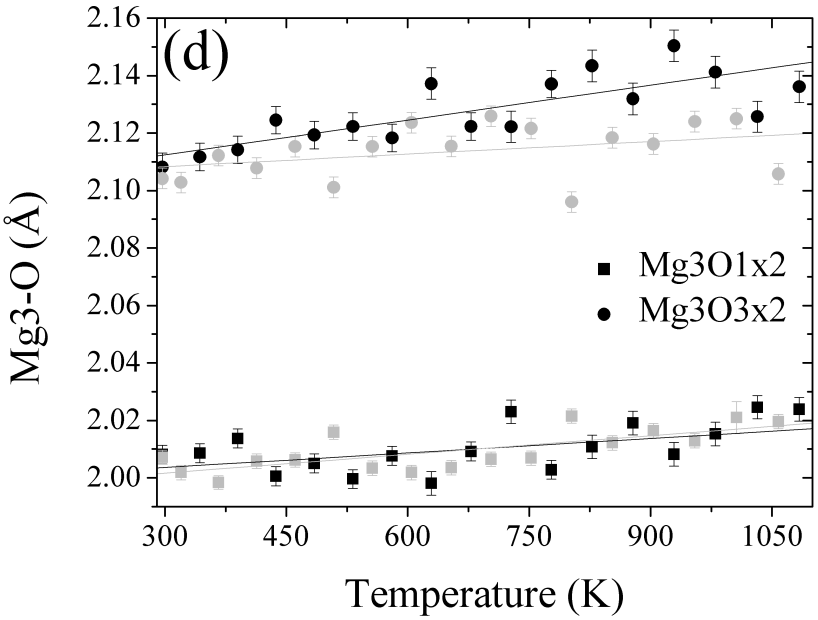
Appendix 3. Temperature dependencies of interatomic distances, angles in polyhedral volumes in wadsleyite structure.

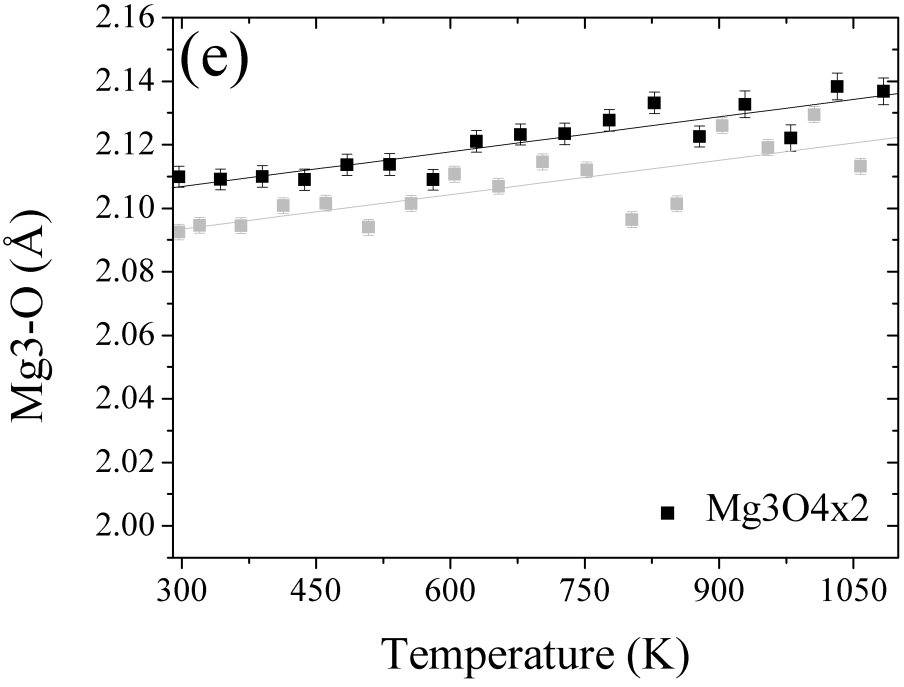
Figure A.3.1. Temperature dependencies of selected interatomic distances in wadsleyite structure (a–e) and temperature dependences of polyhedral volumes at selected temperatures (f). Lines in all dependencies are linear fits and are presented as guides to the eye. Black and grey symbols display distances for z626 and z627, respectively.


(a)
Mg1-O (Å)
Temperature (K)
Mg1O4x4
Mg1O3x2
2.18
2.16
2.14
2.12
2.10
2.08
2.06
2.04
2.02
300
450
600
750
900
1050

z


(c)
Mg2-O (Å)
Temperature (K)
Mg2O2x1
2.16
2.14
2.12
2.10
2.08
2.06
2.04
2.02
2.00
300
450
600
750
900
1050


(d)
Mg3-O (Å)
Temperature (K)
Mg3O1x2
Mg3O3x2
2.16
2.14
2.12
2.10
2.08
2.06
2.04
2.02
2.00
300
450
600
750
900
1050


(e)
Mg3-O (Å)
Temperature (K)
Mg3O4x2
2.16
2.14
2.12
2.10
2.08
2.06
2.04
2.02
2.00
300
450
600
750
900
1050

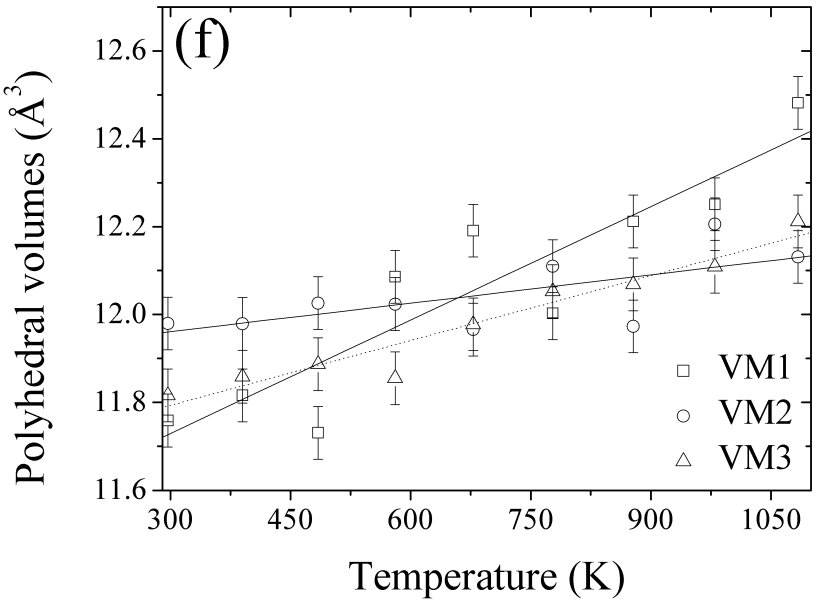
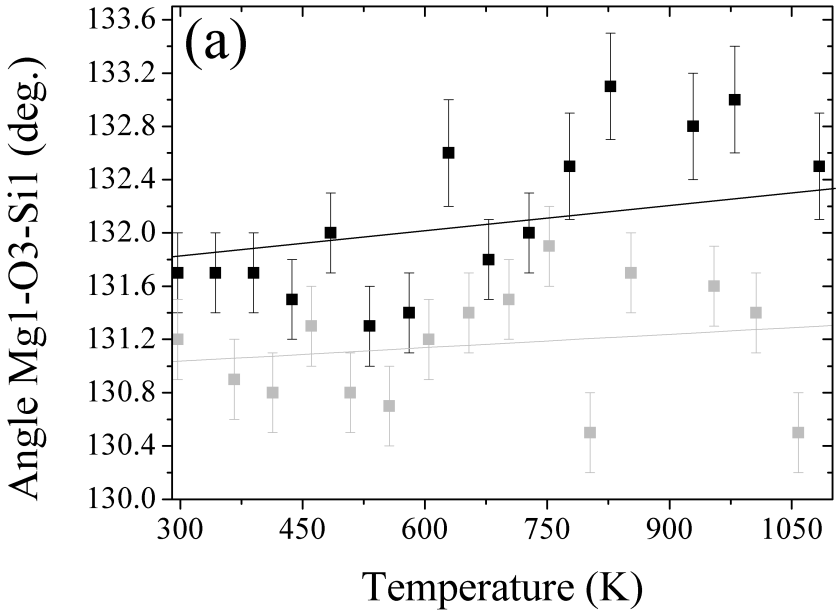
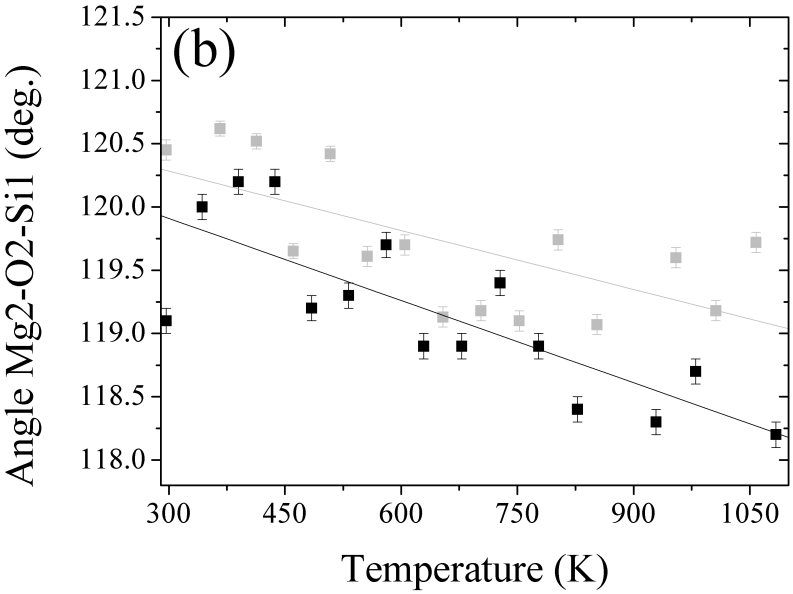
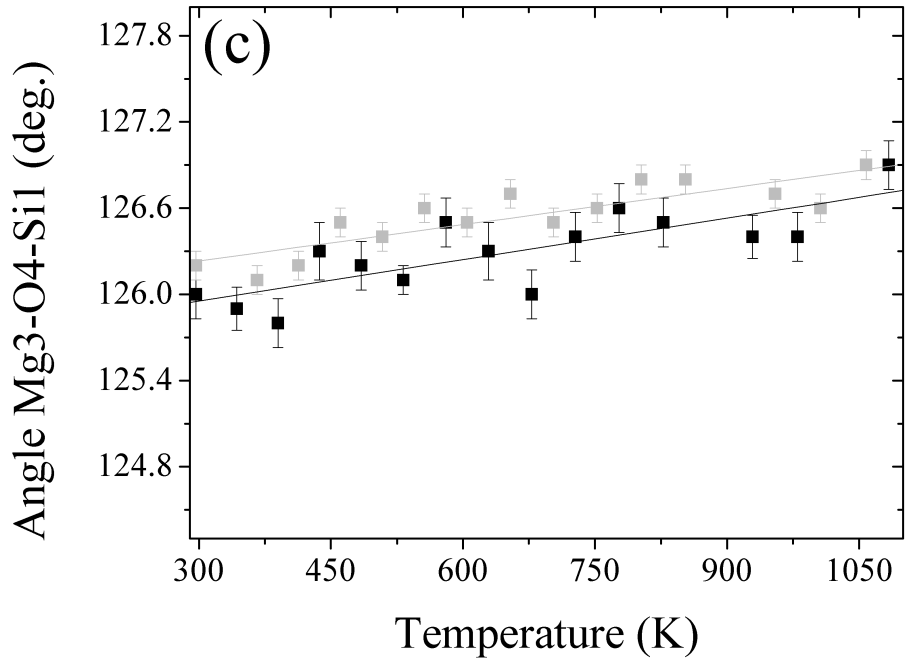
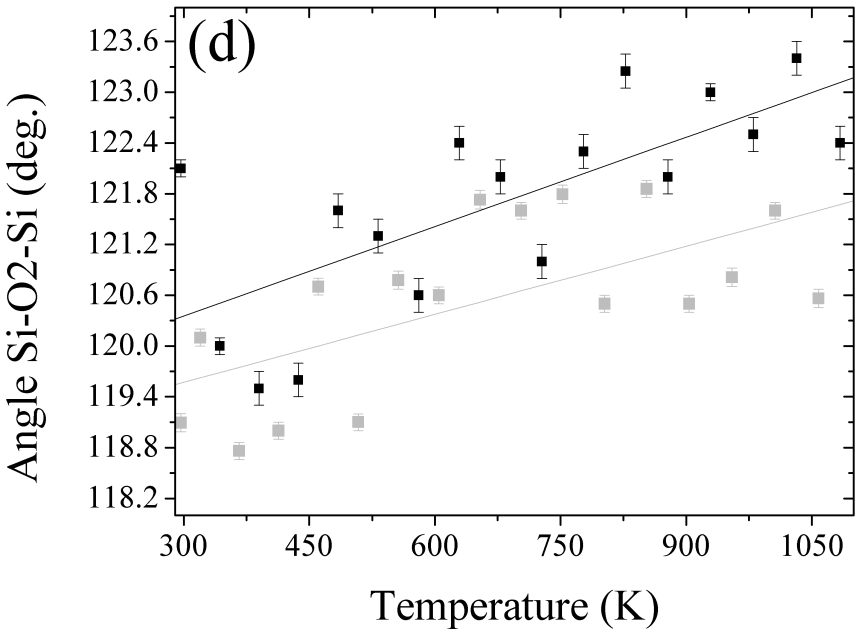


Figure A.3.2. Temperature dependencies of selected angles in wadsleyite structure. Lines in all dependencies are linear fits and are presented as guides to the eye. Black and grey symbols display angles for z626 and z627, respectively.




(b)
Angle Mg2-O2-Si1 (deg.)
121.5
121.0
120.5
120.0
119.5
119.0
118.5
118.0
300
450
600
750
900
1050
Temperature (K)


(c)
Angle Mg3-O4-Si1 (deg.)
127.8
127.2
126.6
126.0
125.4
124.8
300
450
600
750
900
1050
Temperature (K)


(d)
Angle Si-O2-Si (deg.)
123.6
123.0
122.4
121.8
121.2
120.6
120.0
119.4
118.8
118.2
300
450
600
750
900
1050
Temperature (K)