Table S1. Profile parameters for the studied space groups without constraints.

Space group		$\boldsymbol{Ia\bar{3}d}$	$\boldsymbol{R\bar{3}c}$	***Fddd***	$\boldsymbol{C2/c}$	$\boldsymbol{I\bar{1}}$	$\boldsymbol{R\bar{3}}$	$\boldsymbol{I4_1/a}$
SCOR		2.1657	2.1658	2.1779	2.1751	3.9389	2.1440	2.1189
Overall scale f. ($\times 10^{-6}$)		40(1)*	13.3(9)	8.4(5)	16.2(8)	77(7)	13(1)	29(2)
Eta (p-v) or m(p-vii)		0.62(8)	0.66(8)	0.65(9)	0.2(1)	0.4(2)	0.68(8)	0.67(8)
Overall temp. factor		-1.8(2)	-2.1(2)	-2.1(2)	-0.2(2)	0.4(2)	-2.0(3)	-1.9(2)
Halfwidth parameters	U	0.52(6)	0.53(7)	0.48(7)	0.14(2)	0.11(3)	0.49(7)	0.51(6)
	V	-0.10(3)	-0.11(3)	-0.12(3)	-0.12(2)	-0.09(3)	-0.10(3)	-0.11(3)
	W	0.016(3)	0.016(3)	0.018(3)	0.037(4)	0.028(7)	0.016(3)	0.015(3)
Preferred orientation		0.24(7)	0.38(7)	0.22(8)	0.71(3)	-0.59(8)	0.46(8)	0.37(6)
Asymmetry parameters	As 1	0.18(1)	0.18(1)	0.18(2)	0.09(1)	0.05(2)	0.17(1)	0.18(1)
	As 2	0.100(4)	0.100(4)	0.107(5)	0.052(5)	0.034(8)	0.099(4)	0.102(4)
X parameter		0.009(1)	0.009(4)	0.009(1)	0.009(2)	0.002(4)	0.008(1)	0.009(1)
Zero-point		0.026(6)	0.028(6)	0.026(6)	0.023(4)	0.02(1)	0.025(6)	0.024(6)
N° of varied param.		116	132	141	171[1]	139[2]	153	140

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number

[1]-For the monoclinic *C2/c* s.g., number of varied parameters for chlorite was, in this case, decreased to 29 because the maximum of total varied parameters could be 200 [21]

[2]-For the triclinic $I\bar{1}$ s.g., instead of 100 parameters for the background description, 6 Chebyschev's polynomial parameters were used, and 2θ were omitted from the region, from 4° to 10°.

Table S2. Unit cell dimensions and quantitative contents of garnet and chlorite for the studied space groups without constraints. Calculated 4 × c_0/a_0 parameters and distortion angles (α) for the rhombohedral $R\bar{3}c$ and $R\bar{3}$ s.g.'s, and specific geometry–mathematical transformations [5,6] of the crystallographic axes within $Ia\bar{3}d$, $R\bar{3}c$, $R\bar{3}$, *Fddd*, *C*2/*c*, and $I\bar{1}$ s.g.'s are also presented.

Space group	$Ia\bar{3}d$	$R\bar{3}c$	***Fddd***	***C*2/*c***	$I\bar{1}$	$R\bar{3}$	$I4_1/a$
a_0 (Å)	11.869(1)*	16.790(4)	16.809(6)	16.774(2)	11.873(3)	16.791(4)	11.872(3)
b_0 (Å)	11.869(1)	16.790(4)	16.776(8)	11.852(1)	11.852(3)	16.791(4)	11.872(3)
c_0 (Å)	11.869(1)	10.273(3)	11.857(4)	11.879(1)	11.936(3)	10.272(3)	11.860(5)
$a_0 \times \sqrt{3}/2$ (Å)	10.279(1)	/	/	/	/	/	/
$a_0 \times \sqrt{2}$ (Å)	16.785(1)	/	/	/	16.791(3)	/	/
$b_0 \times \sqrt{2}$ (Å)	/	/	/	16.761(1)	16.761(3)	/	/
$c_0 \times \sqrt{2}$ (Å)	/	/	16.768(4)	16.799(1)	16.880(3)	/	/
$\Delta\lvert a_0 - b_0\rvert$	/	/	0.033(7)	0.013(2)	0.030(3)	/	/
$\Delta\lvert a_0 - c_0\rvert$	/	/	0.041(5)	0.025(2)	0.089(3)	/	/
$\Delta\lvert b_0 - c_0\rvert$	/	/	0.008(6)	0.038(1)	0.119(3)	/	/
$a_0 / \sqrt{2}$ (Å)	/	11.872(4)	11.886(6)	11.861(2)	/	11.873(4)	/
$b_0 / \sqrt{2}$ (Å)	/	/	11.862(8)	/	/	/	/
$c_0 / \sqrt{3}/2$ (Å)	/	11.862(3)	/	/	/	11.861(3)	/
$\Delta\lvert a_0 - b_0\rvert$	/	/	0.024(7)	0.009(2)	0.021(3)	/	/
$\Delta\lvert a_0 - c_0\rvert$	/	0.010(4)	0.029(5)	0.018(2)	0.063(3)	0.012(4)	0.010(4)
$\Delta\lvert b_0 - c_0\rvert$	/	/	0.005(6)	0.027(1)	0.084(3)	/	/
$\langle a_0 \rangle$	11.869(1)	11.867(4)	11.868(6)	11.864(1)	11.887(3)	11.869(4)	11.868(4)
4 × c_0/a_0	/	2.4474	/	/	/	2.4470	/
α (°)	/	60.036	/	/	/	60.044	/
α_0 (°)	90	90	90	90	89.77(2)	90	90
β_0 (°)	90	90	90	134.55(5)	90.45(2)	90	90
γ_0 (°)	90	120	90	90	90.14(2)	120	90
V_0 (Å^3)	1671.9(3)	2508(1)	3344(2)	1683.1(3)	1679.6(8)	2508(1)	1671.7(9)
garnet (in %)	91(5)	91(9)	89(8)	86(5)	75(9)	88(10)	90(9)
chlorite (in %)	9(1)	9(2)	11(2)	14(1)	25(4)	12(2)	10(2)

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.

Table S3. Calculated Al *sof's* (in %) and selected Si-O, *Y*-O, and Ca-O distances (in Å) for the studied space groups without constraints.

Space group	$Ia\bar{3}d$	$R\bar{3}c$	$Fddd$	$C2/c$	$I\bar{1}$	$R\bar{3}$	$I4_1/a$
Al1	104(1)*	113(17)	114(11)	99(11)	100(31)	122(5)	104(1)
Al2	/	101(6)	92(11)	114(10)	91(33)	103(7)	105(1)
Al3	/	/	/	97(11)	93(34)	103(3)	/
Al4	/	/	/	108(10)	86(34)I	103(3)	/
Al5	/	/	/	/	125(29)	/	/
Al6	/	/	/	/	91(32)	/	/
Al7	/	/	/	/	89(29)	/	/
Al8	/	/	/	/	90(30)	/	/
ΔAl	0	12(12)	22(11)	17(10)	39(32)	19(5)	1(1)
<Al>	104(1)	107(12)	102(11)	104(10)	96(32)	108(4)	104(1)
$Al_{<a0>}$	90.5	91.5	91.0	93.0	81.5	90.5	91.0
Al_{V0}	90.8	90.7	91.9	77.7	81.8	90.7	91.0
Si1-O	1.622(5)	1.63(2)	1.61(6)	1.65(6)	1.60(12)	1.66(6)	1.55(3)
Si2-O	/	/	1.64(8)	1.59(6)	1.58(12)	1.60(6)	1.62(3)
Si3-O	/	/	/	1.65(7)	1.69(12)	/	1.67(3)
Si4-O	/	/	/	1.64(6)	1.59(12)	/	/
Si5-O	/	/	/	/	1.65(11)	/	/
Si6-O	/	/	/	/	1.73(12)	/	/
<Si–O>	1.622(5)	1.63(2)	1.62(7)	1.63(6)	1.64(12)	1.63(6)	1.61(3)
*Y*1-O	1.950(5)	1.87(2)	1.91(7)	1.95(6)	1.92(10)	1.89(5)	1.97(3)
*Y*2-O	/	1.99(2)	1.99(7)	1.96(6)	2.00(10)	1.90(5)	1.91(3)
*Y*3-O	/	/	/	2.02(6)	2.14(10)	2.00(5)	/
*Y*4-O	/	/	/	1.96(5)	2.01(12)	1.97(5)	/
*Y*5-O	/	/	/	/	1.87(10)	/	/
*Y*6-O	/	/	/	/	2.00(10)	/	/
*Y*7-O	/	/	/	/	1.98(11)	/	/
*Y*8-O	/	/	/	/	1.98(11)	/	/
Δ*Y*	/	0.12(2)	0.08(7)	0.07(6)	0.27(10)	0.11(5)	0.06(3)
<*Y*–O>	1.950(5)	1.93(2)	1.95(7)	1.97(6)	1.99(10)	1.94(5)	1.94(3)
Ca1-O	2.490(5)	2.45(2)	2.48(7)	2.50(6)	2.42(11)	2.44(5)	2.40(4)
Ca2-O	2.357(5)	2.41(2)	2.46(6)	2.50(6)	2.46(12)	2.42(6)	2.47(3)
Ca3-O	/	/	2.40(7)	2.39(6)	2.33(12)	/	/
Ca4-O	/	/	/	2.38(6)	2.43(11)	/	/
Ca5-O	/	/	/	/	2.45(11)	/	/
Ca6-O	/	/	/	/	2.40(12)	/	/
<Ca–O>	2.424(5)	2.43(2)	2.45(7)	2.44(6)	2.42(12)	2.43(6)	2.44(4)
<*D*–O>	2.105(5)	2.09(2)	2.12(7)	2.12(6)	2.12(12)	2.11(6)	2.10(3)

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.
<*D*–O> = {<Si–O> + <*Y*–O> + 2 × <Ca–O>}/4

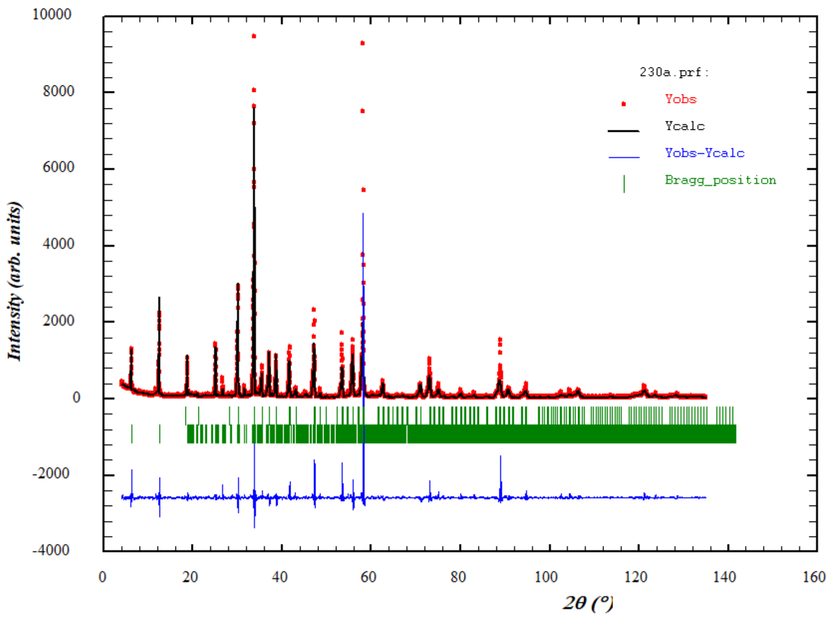

Figure S1. Final Rietveld plot for the $Ia\bar{3}d$ space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

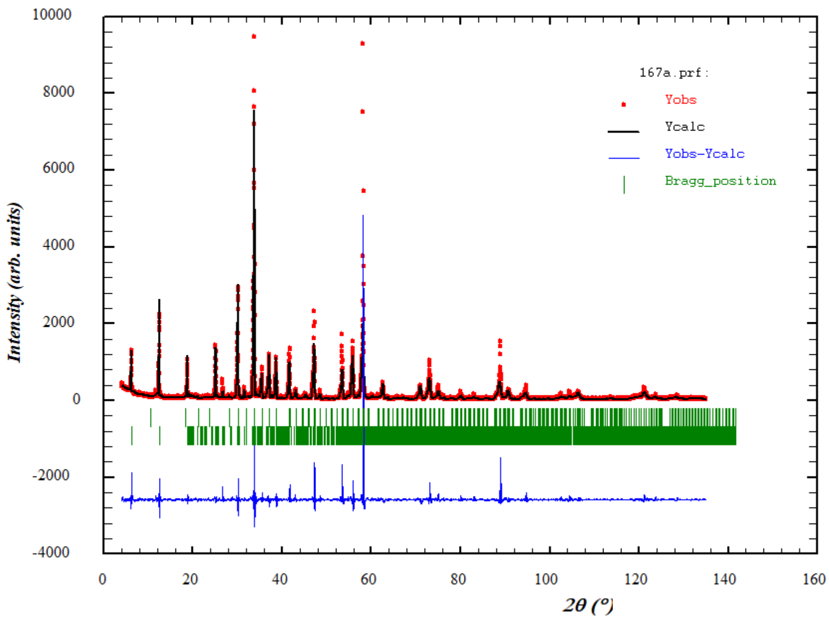

Figure S2. Final Rietveld plot for the $R\bar{3}c$ space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

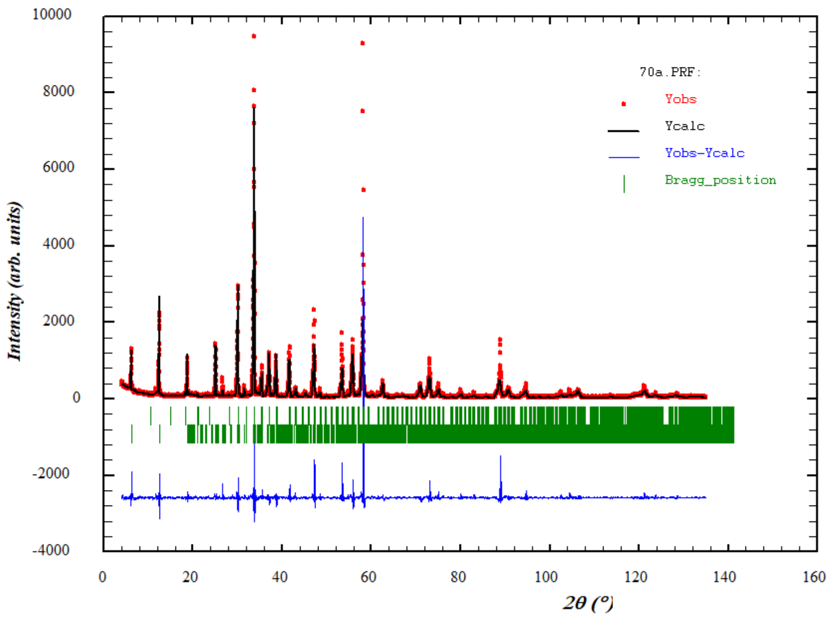

Figure S3. Final Rietveld plot for the *Fddd* space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

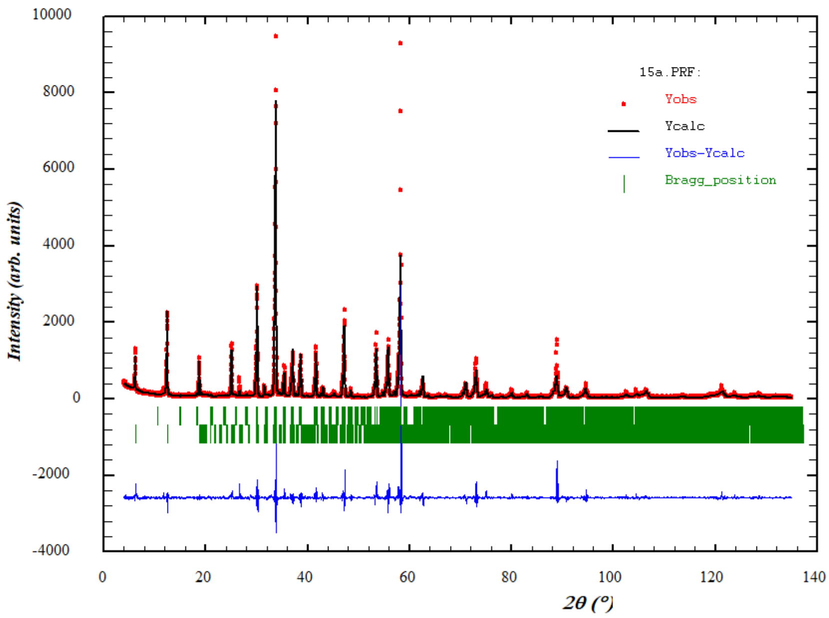

Figure S4. Final Rietveld plot for the *C2/c* space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

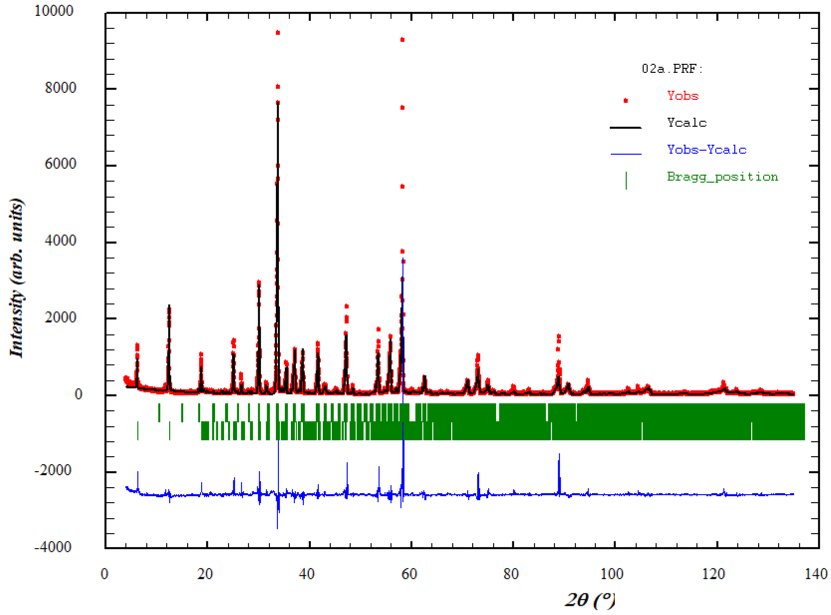

Figure S5. Final Rietveld plot for the $I\bar{1}$ space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

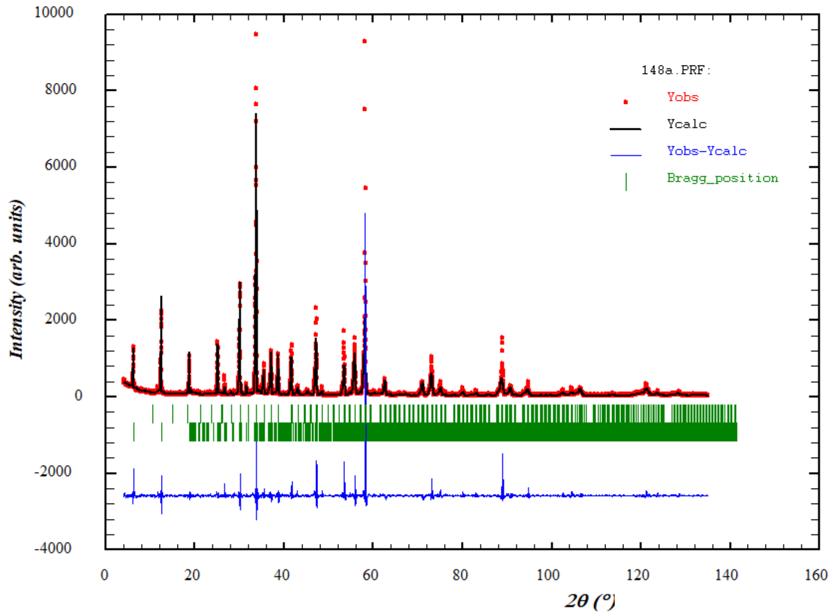

Figure S6. Final Rietveld plot for the $R\bar{3}$ space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

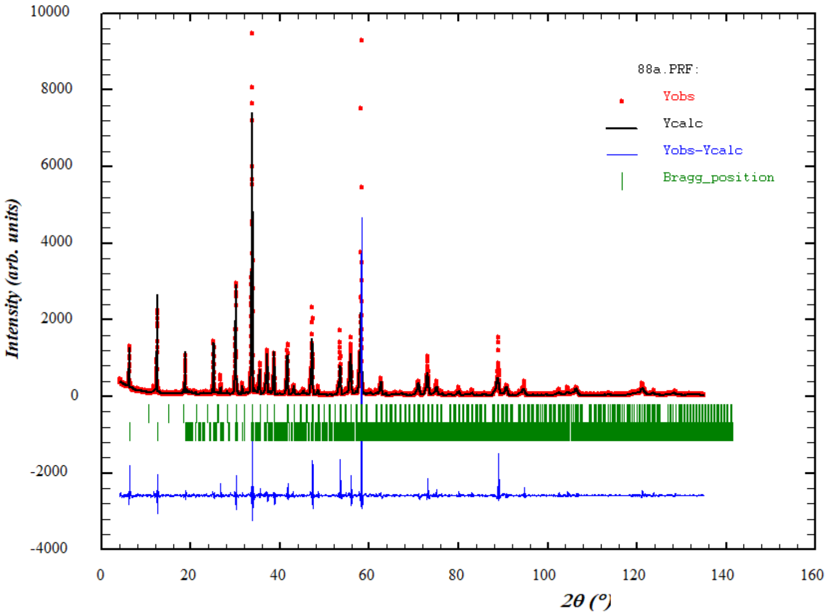

Figure S7. Final Rietveld plot for the *I4₁/a* space group without constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

Table S4. Profile parameters for the studied space groups with constraints.

Space group		$\boldsymbol{Ia\bar{3}d}$	$\boldsymbol{R\bar{3}c}$	***Fddd***	$\boldsymbol{C2/c}$	$\boldsymbol{I\bar{1}}$	$\boldsymbol{R\bar{3}}$	$\boldsymbol{I4_1/a}$
SCOR		2.2613	2.1696	2.2627	2.6920	3.9769	2.2691	2.1482
Overall scale f. ($\times 10^{-6}$)		39(2)*	17(1)	9.7(6)	15(1)	59(5)	47(6)	30(2)
Eta (p-v) or m(p-vii)		0.61(9)	0.62(8)	0.66(9)	0.4(1)	0.5(2)	0.66(9)	0.70(8)
Overall temp. factor		-1.8(2)	-2.0(2)	-1.8(2)	-0.7(2)	0.5(2)	-2.0(3)	-1.6(2)
Halfwidth parameters	U	0.52(7)	0.53(7)	0.47(8)	0.19(4)	0.13(4)	0.53(7)	0.50(7)
	V	-0.10(3)	-0.11(3)	-0.10(3)	-0.14(3)	-0.10(4)	-0.11(3)	-0.09(3)
	W	0.015(3)	0.016(3)	0.017(4)	0.039(5)	0.027(8)	0.016(3)	0.014(3)
Preferred orientation		0.02(6)	0.07(5)	0.03(7)	0.75(4)	-0.35(7)	0.14(6)	0.40(5)
Asymmetry parameters	As 1	0.17(1)	0.18(1)	0.17(2)	0.09(2)	0.05(2)	0.17(1)	0.17(1)
	As 2	0.099(5)	0.102(4)	0.103(5)	0.054(6)	0.030(8)	0.098(5)	0.098(5)
X parameter		0.009(1)	0.009(1)	0.009(1)	0.007(2)	-0.001(4)	-0.002(4)	0.008(1)
Zero-point		0.024(6)	0.026(6)	0.024(6)	0.018(6)	0.023(9)	0.025(6)	0.021(6)
N^{o} of varied param.		115	131	140	169[1]	135[2]	151	139

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.

[1]-For the monoclinic *C2/c* s.g., number of varied parameters for chlorite was, in this case, decreased to 31 because the maximum total varied parameters could be 200 [21]

[2]-For the triclinic $I\bar{1}$ s.g., instead of 100 parameters for the background description, 6 Chebyschev's polynomial parameters were used, and 2θ were omitted from the region from 4° to 10°.

Table S5. Unit cell dimensions and quantitative contents of garnet and chlorite for the studied space groups with constraints. Calculated 4 × c_0/a_0 parameters and distortion angles (α) for the rhombohedral $R\bar{3}c$ and $R\bar{3}$ s.g.'s, and specific geometry–mathematical transformations [5,6] of the crystallographic axes within $Ia\bar{3}d$, $R\bar{3}c$, $R\bar{3}$, *Fddd*, *C*2/*c*, and $I\bar{1}$ s.g.'s, are also presented.

Space group	$Ia\bar{3}d$	$R\bar{3}c$	***Fddd***	***C*2/*c***	$I\bar{1}$	$R\bar{3}$	$I4_1/a$
a_0 (Å)	11.868(1)*	16.790(5)	16.805(8)	16.775(2)	11.875(3)	16.790(6)	11.869(3)
b_0 (Å)	11.868(1)	16.790(5)	16.778(9)	11.853(2)	11.852(3)	16.790(6)	11.869(3)
c_0 (Å)	11.868(1)	10.273(6)	11.858(6)	11.880(2)	11.931(3)	10.273(6)	11.865(5)
$a_0 \times \sqrt{3}/2$ (Å)	10.278(1)	/	/	/	/	/	/
$a_0 \times \sqrt{2}$ (Å)	16.784(1)	/	/	/	16.794(3)	/	/
$b_0 \times \sqrt{2}$ (Å)	/	/	/	16.763(2)	16.761(3)	/	/
$c_0 \times \sqrt{2}$ (Å)	/	/	16.770(6)	16.801(2)	16.873(3)	/	/
$\Delta\lvert a_0 - b_0\rvert$	/	/	0.027(8)	0.012(2)	0.033(3)	/	/
$\Delta\lvert a_0 - c_0\rvert$	/	/	0.035(7)	0.026(2)	0.079(3)	/	/
$\Delta\lvert b_0 - c_0\rvert$	/	/	0.008(8)	0.038(2)	0.112(3)	/	/
$a_0 / \sqrt{2}$ (Å)	/	11.872(5)	11.883(8)	11.862(2)	/	11.872(6)	/
$b_0 / \sqrt{2}$ (Å)	/	/	11.864(9)	/	/	/	/
$c_0 / \sqrt{3}/2$ (Å)	/	11.862(6)	/	/	/	11.862(6)	/
$\Delta\lvert a_0 - b_0\rvert$	/	/	0.019(8)	0.009(2)	0.023(3)	/	/
$\Delta\lvert a_0 - c_0\rvert$	/	0.010(6)	0.025(7)	0.018(2)	0.056(3)	0.010(6)	0.004(4)
$\Delta\lvert b_0 - c_0\rvert$	/	/	0.006(8)	0.027(2)	0.079(3)	/	/
$\langle a_0\rangle$	11.868(1)	11.867(6)	11.868(8)	11.865(2)	11.886(3)	11.867(6)	11.868(4)
$4 \times c_0/a_0$	/	2.4474	/	/	/	2.4474	/
α (°)	/	60.036	/	/	/	60.036	/
α_0 (°)	90	90	90	90	89.76(2)	90	90
β_0 (°)	90	90	90	134.54(1)	90.45(2)	90	90
γ_0 (°)	90	120	90	90	90.14(2)	120	90
V_0 (Å^3)	1671.8(3)	2508(2)	3343(3)	1683.6(5)	1679.1(8)	2508(2)	1671.5(9)
garnet (in %)	86(5)	88(7)	88(7)	86(8)	77(8)	84(7)	91(7)
chlorite (in %)	14(2)	12(2)	12(2)	14(2)	23(4)	16(2)	9(1)

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.

Table S6. Calculated Al *sof's* (in %) and selected Si-O, *Y*-O and Ca-O distances (in Å) for the studied space groups with constraints.

Space group	$Ia\bar{3}d$	$R\bar{3}c$	*Fddd*	*C*2/*c*	$I\bar{1}$	$R\bar{3}$	$I4_1/a$
Al1	90(0)*	101(3)	97(13)	123(8)	93(24)	83(2)	88(6)
Al2	/	79(3)	83(13)	57(8)	87(24)	97(2)	92(6)
Al3	/	/	/	86(8)	90(21)	90(8)	/
Al4	/	/	/	94(8)	90(21)	90(8)	/
Al5	/	/	/	/	112(11)	/	/
Al6	/	/	/	/	68(11)	/	/
Al7	/	/	/	/	88(19)	/	/
Al8	/	/	/	/	92(19)	/	/
ΔAl	0	22(3)	14(13)	66(8)	44(11)	14(2)	4(6)
<Al>	90(0)	90(3)	90(13)	90(8)	90(19)	90(5)	90(6)
$Al_{<a0>}$	91.0	91.5	91.0	92.5	82.0	91.5	91.0
Al_{V0}	90.9	90.7	91.3	77.1	82.4	90.7	91.3
Si1-O	1.640(4)	1.642(7)	1.644(6)	1.656(8)	1.644(7)	1.645(7)	1.647(6)
Si2-O	/	/	1.644(7)	1.648(8)	1.644(8)	1.644(8)	1.649(5)
Si3-O	/	/	/	1.65(1)	1.644(7)	/	1.650(7)
Si4-O	/	/	/	1.655(8)	1.644(8)	/	/
Si5-O	/	/	/	/	1.645(8)	/	/
Si6-O	/	/	/	/	1.646(7)	/	/
<Si–O>	1.640(4)	1.642(7)	1.644(6)	1.652(8)	1.644(8)	1.644(8)	1.649(6)
*Y*1-O	1.935(4)	1.900(6)	1.905(6)	1.922(7)	1.966(6)	1.939(7)	1.972(7)
*Y*2-O	/	1.960(6)	1.980(6)	1.911(7)	1.953(6)	1.906(6)	1.918(6)
*Y*3-O	/	/	/	2.062(9)	1.960(7)	1.988(7)	/
*Y*4-O	/	/	/	1.902(6)	1.989(7)	1.944(6)	/
*Y*5-O	/	/	/	/	1.894(6)	/	/
*Y*6-O	/	/	/	/	1.910(6)	/	/
*Y*7-O	/	/	/	/	1.982(7)	/	/
*Y*8-O	/	/	/	/	2.001(7)	/	/
Δ*Y*	/	0.060(6)	0.075(6)	0.160(8)	0.107(6)	0.082(6)	0.054(6)
<*Y*–O>	1.935(4)	1.930(6)	1.942(6)	1.949(7)	1.957(6)	1.944(6)	1.945(6)
Ca1-O	2.495(4)	2.408(6)	2.410(5)	2.414(7)	2.405(6)	2.408(7)	2.410(7)
Ca2-O	2.332(4)	2.408(6)	2.410(5)	2.416(7)	2.406(7)	2.408(7)	2.411(6)
Ca3-O	/	/	2.408(6)	2.412(9)	2.404(7)	/	/
Ca4-O	/	/	/	2.409(8)	2.406(6)	/	/
Ca5-O	/	/	/	/	2.405(6)	/	/
Ca6-O	/	/	/	/	2.404(6)	/	/
<Ca–O>	2.414(4)	2.408(6)	2.409(5)	2.413(8)	2.405(6)	2.408(7)	2.410(6)
<*D*–O>	2.100(4)	2.097(6)	2.101(6)	2.107(8)	2.103(6)	2.101(7)	2.104(6)

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.
<*D*–O> = {<Si–O> + <*Y*–O> + 2 × <Ca–O>}/4

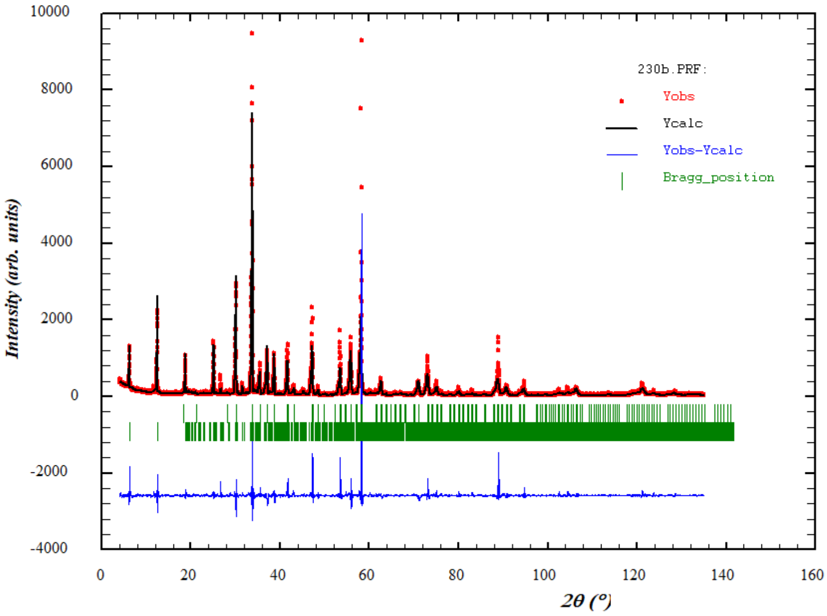

Figure S8. Final Rietveld plot for the $Ia\bar{3}d$ space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

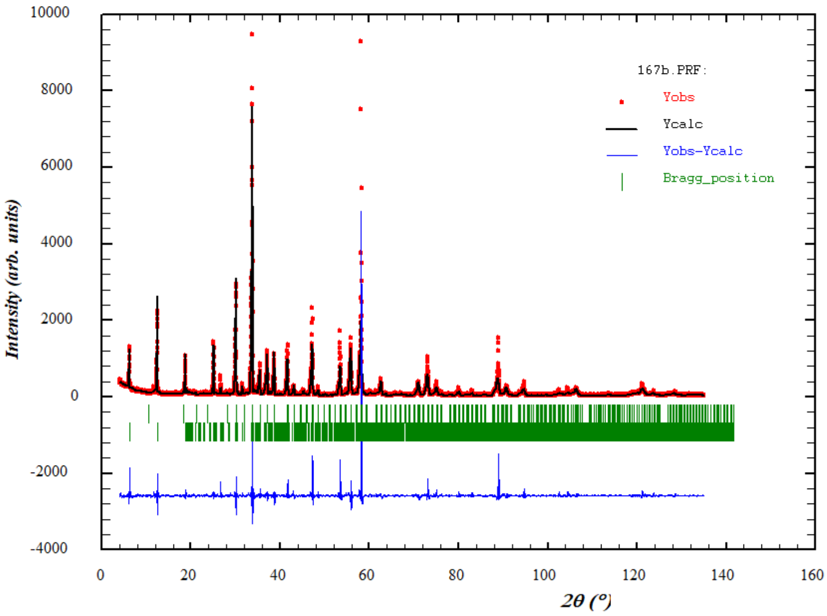

Figure S9. Final Rietveld plot for the $R\bar{3}c$ space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

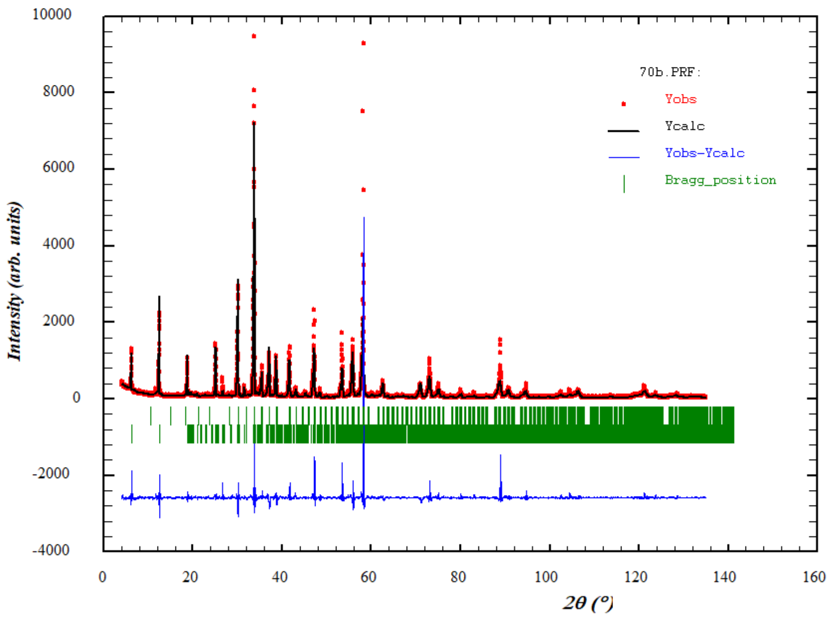

Figure S10. Final Rietveld plot for the *Fddd* space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

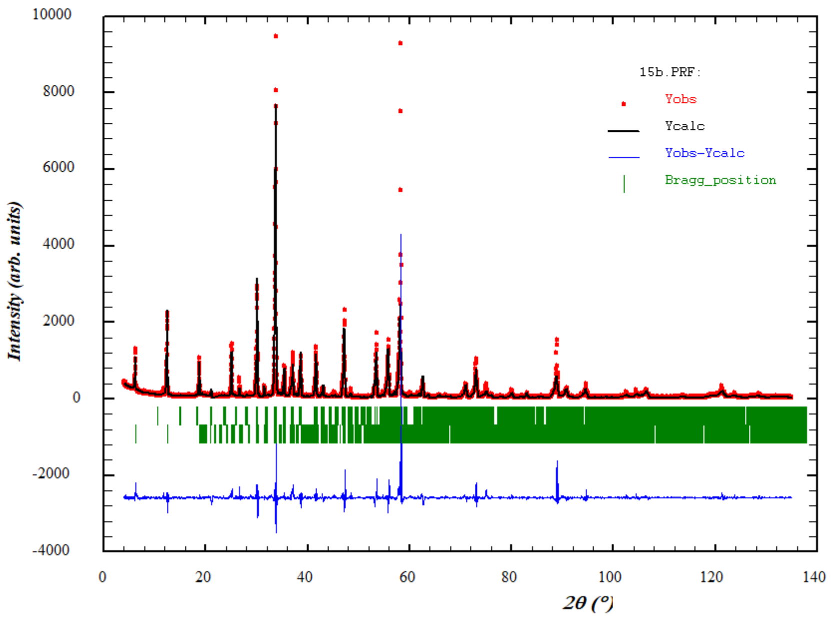

Figure S11. Final Rietveld plot for the *C2/c* space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

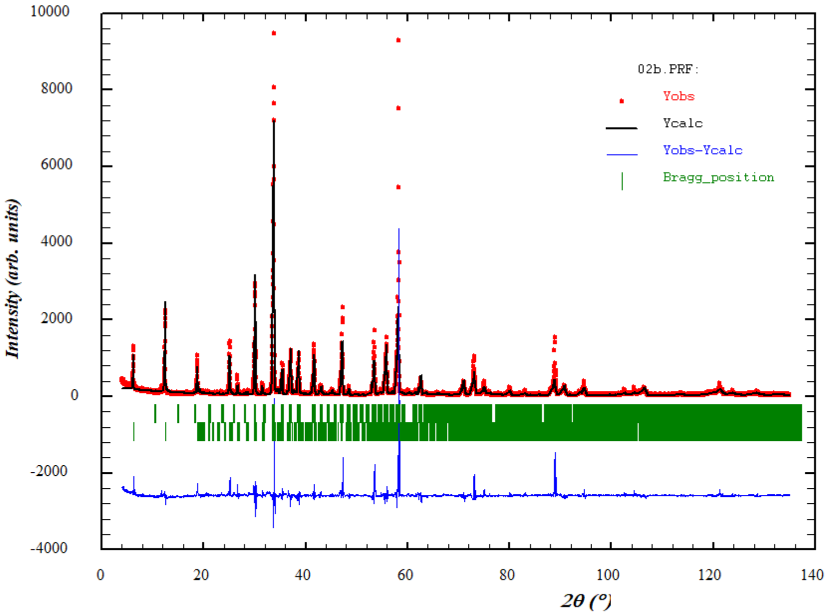

Figure S12. Final Rietveld plot for the $I\bar{1}$ space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

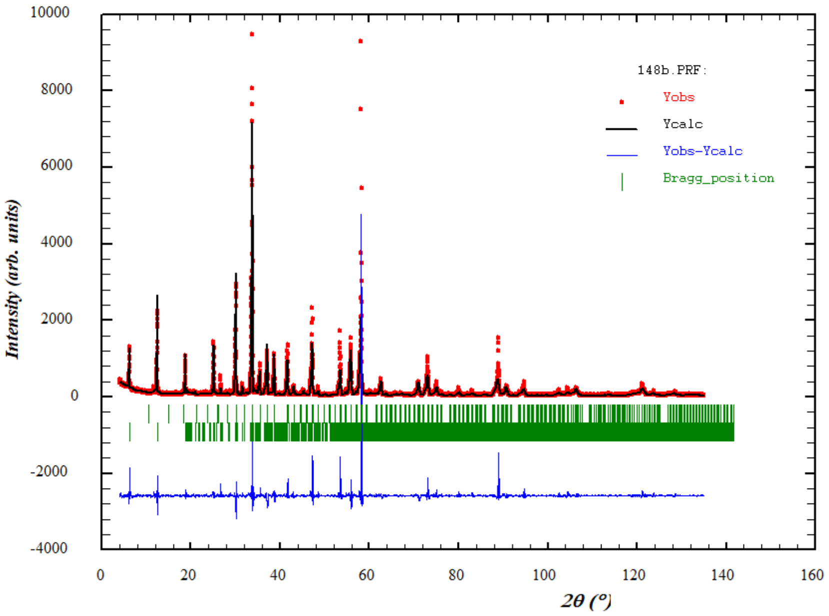

Figure S13. Final Rietveld plot for the $R\bar{3}$ space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

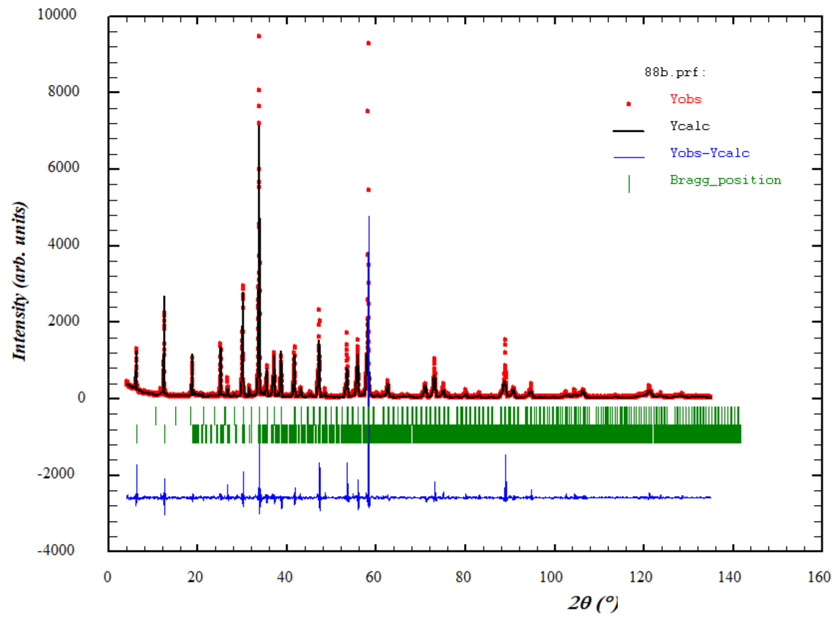

Figure S14. Final Rietveld plot for the *I4₁/a* space group with constraints. Observed intensities (Y_{obs}) were presented with red color, calculated intensities (Y_{calc}) were presented with black color, and differences between observed and calculated intensities (Y_{obs}-Y_{calc}) were presented with blue color. Reflection (Bragg) positions were presented with green vertical bars; upper row: garnet; lower row: chlorite.

Table S7. Selected distances (in Å) and angles (in °) for the orthorhombic *Fddd* space group (without[a] and with[b] constraints).

distances		***Fddd***^{a}	***Fddd***^{b}	**expected**$^{\#}$	angles		***Fddd***^{a}	***Fddd***^{b}	**expected**$^{\#}$
Si(1)–O(2)	2$^{\$}$	1.70(6)*	1.644(6)						
Si(1)–O(4)	2	1.52(6)	1.644(6)						
<Si(1)–O>		1.61(6)	1.644(6)	1.645					
O(2)–O(2)	1	2.54(8)	2.562(7)		O(2)–Si(1)–O(2)	1	97(5)	102.4(5)	
O(2)–O(4)	2	2.62(10)	2.750(7)		O(2)–Si(1)–O(4)	2	109(6)	113.5(5)	
O(2)–O(4)	2	2.67(8)	2.732(7)		O(2)–Si(1)–O(4)	2	112(6)	112.4(5)	
O(4)–O(4)	1	2.57(9)	2.572(5)		O(4)–Si(1)–O(4)	1	116(7)	103.0(5)	
<O–O>		2.62(9)	2.683(7)	2.686	<O–Si(1)–O>		109(6)	109.5(5)	109.54
Si(2)–O(1)	1	1.61(8)	1.646(7)						
Si(2)–O(3)	1	1.71(5)	1.642(6)						
Si(2)–O(5)	1	1.61(11)	1.645(8)						
Si(2)–O(6)	1	1.61(6)	1.643(7)						
<Si(2)–O>		1.64(8)	1.644(7)	1.645					
<Si–O>		1.62(7)	1.644(6)	1.645					
O(1)–O(3)	1	2.88(8)	2.823(7)		O(1)–Si(2)–O(3)	1	120(5)	118.3(5)	
O(1)–O(5)	1	2.49(13)	2.650(8)		O(1)–Si(2)–O(5)	1	101(8)	107.3(6)	
O(1)–O(6)	1	2.42(8)	2.490(9)		O(1)–Si(2)–O(6)	1	98(6)	98.4(6)	
O(3)–O(5)	1	2.67(9)	2.613(8)		O(3)–Si(2)–O(5)	1	106(6)	105.3(6)	
O(3)–O(6)	1	2.87(6)	2.861(7)		O(3)–Si(2)–O(6)	1	120(5)	121.1(5)	
O(5)–O(6)	1	2.64(10)	2.613(9)		O(5)–Si(2)–O(6)	1	110(7)	105.2(6)	
<O–O>		2.66(9)	2.675(8)	2.686	<O–Si(2)–O>		109(6)	109.3(6)	109.54
<O–O>$_{tet}$		2.64(9)	2.679(8)	2.686	<O–Si–O>		109(6)	109.4(6)	109.54
Y(1)–O(1)	2	1.95(6)	1.974(6)						
Y(1)–O(2)	2	1.95(9)	1.934(6)						
Y(1)–O(3)	2	1.83(5)	1.806(5)						
<*Y*(1)–O>		1.91(7)	1.905(6)	1.931					
O(1)–O(2)	2	2.61(10)	2.726(8)		O(1)–*Y*(1)–O(2)	2	84(5)	88.4(4)	
O(1)–O(2)	2	2.91(10)	2.800(8)		O(1)–*Y*(1)–O(2)	2	96(6)	91.6(4)	
O(1)–O(3)	2	2.63(7)	2.652(7)		O(1)–*Y*(1)–O(3)	2	88(4)	89.0(4)	
O(1)–O(3)	2	2.73(8)	2.700(7)		O(1)–*Y*(1)–O(3)	2	92(4)	91.0(4)	
O(2)–O(3)	2	2.66(12)	2.631(8)		O(2)–*Y*(1)–O(3)	2	89(6)	89.3(4)	
O(2)–O(3)	2	2.70(7)	2.661(7)		O(2)–*Y*(1)–O(3)	2	91(4)	90.7(4)	
<O–O>		2.71(9)	2.695(8)	2.731	<O–*Y*(1)–O>		90(5)	90.0(4)	90.0
Y(2)–O(4)	2	1.93(5)	1.943(6)						
Y(2)–O(5)	2	2.03(9)	2.013(6)						
Y(2)–O(6)	2	2.00(6)	1.983(7)						
<*Y*(2)–O>		1.99(7)	1.980(6)	1.931					
<*Y*–O>		1.95(7)	1.942(6)	1.931					
O(4)–O(5)	2	2.71(8)	2.749(8)		O(4)–*Y*(2)–O(5)	2	86(4)	88.0(4)	
O(4)–O(5)	2	2.89(11)	2.847(8)		O(4)–*Y*(2)–O(5)	2	94(6)	92.0(4)	
O(4)–O(6)	2	2.90(7)	2.817(8)		O(4)–*Y*(2)–O(6)	2	95(4)	91.7(4)	
O(4)–O(6)	2	2.65(8)	2.735(8)		O(4)–*Y*(2)–O(6)	2	85(4)	88.3(4)	
O(5)–O(6)	2	2.80(9)	2.740(9)		O(5)–*Y*(2)–O(6)	2	88(5)	86.6(4)	
O(5)–O(6)	2	2.89(11)	2.909(8)		O(5)–*Y*(2)–O(6)	2	92(5)	93.4(4)	
<O–O>		2.81(9)	2.800(8)	2.731	<O–*Y*(2)–O>		90(5)	90.0(4)	90.0
<O–O>$_{oct}$		2.76(9)	2.748(8)	2.731	<O–*Y*–O>		90(5)	90.0(4)	90.0
Ca(1)–O(1)	4	2.63(8)	2.496(5)						
Ca(1)–O(2)	4	2.33(6)	2.323(5)						
<Ca(1)–O>		2.48(7)	2.410(5)	2.406					
O(1)–O(1)	2	2.91(7)	2.903(7)		O(1)–Ca(1)–O(1)	2	67(3)	71.1(3)	

O(1)–O(1)	2	4.45(12)	4.125(7)		O(1)–Ca(1)–O(1)	2	115(5)	111.5(3)	
O(1)–O(2)	4	3.10(12)	2.943(8)		O(1)–Ca(1)–O(2)	4	77(4)	75.2(3)	
O(1)–O(2)	4	3.53(9)	3.430(8)		O(1)–Ca(1)–O(2)	4	91(4)	90.7(3)	
O(1)–O(2)	4	2.91(10)	2.800(8)		O(1)–Ca(1)–O(2)	4	71(4)	71.0(3)	
O(2)–O(2)	2	2.54(8)	2.562(7)		O(2)–Ca(1)–O(2)	2	66(3)	66.9(3)	
<O–O>		3.22(10)	3.104(8)	3.103	<O–Ca(1)–O>		81(4)	80.4(3)	80.51
Ca(2)–O(4)	4	2.41(5)	2.326(5)						
Ca(2)–O(6)	4	2.52(6)	2.493(5)						
<Ca(2)–O>		2.46(6)	2.410(5)	2.406					
O(4)–O(4)	2	4.19(7)	3.970(7)		O(4)–Ca(2)–O(4)	2	121(3)	117.2(3)	
O(4)–O(4)	2	2.57(9)	2.572(7)		O(4)–Ca(2)–O(4)	2	65(3)	67.1(3)	
O(4)–O(6)	4	3.45(9)	3.430(8)		O(4)–Ca(2)–O(6)	4	89(3)	90.7(3)	
O(4)–O(6)	4	2.90(7)	2.817(8)		O(4)–Ca(2)–O(6)	4	72(3)	71.5(3)	
O(4)–O(6)	4	3.03(7)	2.946(8)		O(4)–Ca(2)–O(6)	4	76(3)	75.3(3)	
O(6)–O(6)	2	2.93(9)	2.832(7)		O(6)–Ca(2)–O(6)	2	71(3)	69.2(3)	
<O–O>		3.16(8)	3.084(8)	3.103	<O–Ca(2)–O>		81(3)	80.9(3)	80.51
Ca(3)–O(1)	1	2.40(7)	2.326(6)						
Ca(3)–O(2)	1	2.52(8)	2.493(6)						
Ca(3)–O(3)	1	2.32(7)	2.322(6)						
Ca(3)–O(3)	1	2.34(6)	2.490(6)						
Ca(3)–O(4)	1	2.54(7)	2.492(6)						
Ca(3)–O(5)	1	2.30(6)	2.323(6)						
Ca(3)–O(5)	1	2.51(7)	2.494(7)						
Ca(3)–O(6)	1	2.30(7)	2.323(6)						
<Ca(3)–O>		2.40(7)	2.408(6)	2.406					
<Ca–O>		2.45(7)	2.409(5)	2.406					
O(1)–O(2)	1	3.10(12)	2.943(8)		O(1)–Ca(3)–O(2)	1	78(4)	75.2(3)	
O(1)–O(3)	1	2.63(7)	2.652(7)		O(1)–Ca(3)–O(3)	1	67(3)	66.7(3)	
O(1)–O(4)	1	3.42(7)	3.431(8)		O(1)–Ca(3)–O(4)	1	88(3)	90.7(4)	
O(1)–O(5)	1	4.33(9)	4.256(8)		O(1)–Ca(3)–O(5)	1	124(4)	124.0(4)	
O(1)–O(6)	1	2.42(8)	2.490(9)		O(1)–Ca(3)–O(6)	1	62(3)	64.8(3)	
O(2)–O(3)	1	2.70(7)	2.661(7)		O(2)–Ca(3)–O(3)	1	68(3)	67.0(3)	
O(2)–O(3)	1	3.96(8)	4.052(7)		O(2)–Ca(3)–O(3)	1	109(4)	108.8(3)	
O(2)–O(5)	1	2.84(9)	2.856(8)		O(2)–Ca(3)–O(5)	1	69(3)	69.9(3)	
O(2)–O(6)	1	3.42(12)	3.473(8)		O(2)–Ca(3)–O(6)	1	90(5)	92.2(4)	
O(3)–O(3)	1	2.83(9)	3.003(7)		O(3)–Ca(3)–O(3)	1	75(4)	77.1(3)	
O(3)–O(5)	1	2.67(9)	2.613(8)		O(3)–Ca(3)–O(5)	1	70(3)	68.5(3)	
O(3)–O(5)	1	3.50(9)	3.425(8)		O(3)–Ca(3)–O(5)	1	93(4)	90.6(3)	
O(3)–O(4)	1	2.79(8)	2.876(7)		O(3)–Ca(3)–O(4)	1	70(3)	70.5(3)	
O(3)–O(5)	1	3.44(8)	3.519(8)		O(3)–Ca(3)–O(5)	1	96(4)	93.9(3)	
O(4)–O(5)	1	2.89(11)	2.847(8)		O(4)–Ca(3)–O(5)	1	73(4)	72.4(3)	
O(4)–O(6)	1	3.03(7)	2.946(8)		O(4)–Ca(3)–O(6)	1	78(3)	75.3(3)	
O(5)–O(5)	1	2.94(8)	2.995(8)		O(5)–Ca(3)–O(5)	1	75(3)	76.8(3)	
O(5)–O(6)	1	2.89(11)	2.909(8)		O(5)–Ca(3)–O(6)	1	74(4)	74.2(3)	
<O–O>		3.10(9)	3.108(8)	3.103	<O–Ca(3)–O>		81(3)	81.0(3)	80.51
<O–O>$_{dod}$		3.16(9)	3.099(8)	3.103	<O–Ca–O>		81(3)	80.8(3)	80.51
<*D*–O>		2.12(7)	2.101(6)	2.097					

*-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.

$-Frequency of occurrences.

<*D*–O> = {<Si–O> + <*Y*–O> + 2 × <Ca–O>}/4

#-Expected from the calculations for the cubic $Ia\bar{3}d$ s.g. [19].

Table S8. Selected distances among the studied cation sites (in Å) for the orthorhombic *Fddd* space group (without[a] and with[b] constraints).

distances	***Fddd***[a]	***Fddd***[b]	**expected**[#]
Ca(1)-*Y*(1)	3.31799(4)	3.31785(5)	3.317
Ca(2)-*Y*(2)	3.31799(4)	3.31785(5)	3.317
<Ca(3)-*Y*(1)>	3.32(2)	3.332(3)	3.317
<Ca(3)-*Y*(2)>	3.31(2)	3.302(3)	3.317
Ca(1)–Si(1)	3.08(4)	2.968(6)	2.966
Ca(1)–Si(2)	3.62(4)	3.558(5)	3.634
Ca(2)–Si(1)	2.85(4)	2.961(6)	2.966
Ca(2)–Si(2)	3.71(3)	3.749(4)	3.634
<Ca(3)–Si(1)>	3.64(3)	3.642(4)	3.634
<Ca(3)–Si(2)>	3.29(4)	3.292(6)	3.300
Y(1)–Si(1)	3.37(2)	3.319(3)	3.317
<*Y*(1)–Si(2)>	3.32(3)	3.282(4)	3.317
Y(2)–Si(1)	3.27(2)	3.316(3)	3.317
<*Y*(2)–Si(2)>	3.32(4)	3.357(5)	3.317
Ca(1)–Ca(3)	3.66(2)	3.656(3)	3.634
Ca(2)–Ca(3)	3.63(3)	3.626(3)	3.634
<Ca(3)–Ca(3)>	3.61(3)	3.620(5)	3.634
<Si(1)–Si(2)>	3.66(4)	3.652(4)	3.634
<*Y*(1)–*Y*(1)>	5.13922(8)	5.13909(9)	5.138
<*Y*(1)–*Y*(2)>	5.13922(8)	5.13909(9)	5.138
<*Y*(2)–*Y*(2)>	5.13922(8)	5.13909(9)	5.138

[*]-The numbers in parentheses are the *esd's* multiplied with SCOR [26] and refer to the last significant number.
[#]-Expected from the calculations for the cubic $Ia\bar{3}d$ s.g. [19].