Merohedral mechanism twining growth of natural cation-ordered tetragonal grossular

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1. X-Ray Supplementary Data for tetragonal grossular

Table S1. Atom coordinates, equivalent isotropic displacement parameters and sof's for $(H_4O_4)^{4-}$ substituted grossular from Wiluy River, Yakutia, Russia.

Site	Wyckoff	*sof*	*apfu*	*x*	*y*	*z*	U_{eq} (Å²)
			$Ia\bar{3}d$ model				
*X*1	24*c*	1.0	3Ca	½	¾	1/8	0.0102(3)
*Y*1	16*a*	1.0	1.81Al + 0.19Fe	½	½	0	0.0093(4)
*Z*1	24*d*	0.864(6)	2.59Si + 0.41□	½	¾	7/8	0.0065(4)
O1	96*h*	1.0	12O	0.4538(1)	0.6508(1)	0.9623(1)	0.0125(3)
			$I4_1/acd$ model				
*X*1	16*e*	1.0	2Ca	½	¾	5/8	0.0108(3)
*X*2	8*b*	1.0	1Ca	¾	0.12520(7)	½	0.0107(2)
*Y*1	16*c*	1.0	1.81Al + 0.19Fe	½	½	½	0.0092(4)
*Z*1	16*e*	0.853(6)	0.85Si + 0.15□	¾	0.37506(1)	½	0.0068(4)
*Z*2	8*a*	0.878(7)	1.76Si + 0.24□	½	¾	3/8	0.0069(5)
O1	32*g*	1.0	1O	0.5459(1)	0.6509(1)	0.4618(1)	0.0128(4)
O2	32*g*	1.0	1O	0.6506(1)	0.4624(2)	0.5462(1)	0.0133(4)
O3	32*g*	1.0	1O	0.7039(2)	0.2876(1)	0.4008(1)	0.0131(4)
			$I4_1/a$ model				
*X*1	8*e*	1.0	1Ca	½	¾	0.3759(2)	0.0116(3)
*X*2	16*f*	1.0	2Ca	0.37516(6)	0.5004(1)	0.2499(1)	0.0116(2)
*Y*1	8*c*	1.0	0.97Al + 0.03Fe	½	½	½	0.0074(9)
*Y*2	8*d*	1.0	0.87Al + 0.13Fe	¾	¾	¼	0.0124(9)
*Z*1	4*a*	0.868(4)	0.43Si + 0.07□	½	¾	5/8	0.0081(9)
*Z*2	4*b*	0.862(3)	0.43Si + 0.07□	½	¾	1/8	0.0060(9)
*Z*3	16*f*	0.856(8)	1.71Si + 0.29□	0.62505(9)	0.4993(2)	0.2509(2)	0.0075(3)
O1	16*f*	1.0	2O	0.4556(4)	0.6507(3)	0.5381(4)	0.015(1)
O2	16*f*	1.0	2O	0.5989(3)	0.7974(4)	0.2120(3)	0.014(1)
O3	16*f*	1.0	2O	0.7140(4)	0.6011(4)	0.2045(4)	0.015(1)
O4	16*f*	1.0	2O	0.7106(4)	0.4022(4)	0.2972(3)	0.012(1)
O5	16*f*	1.0	2O	0.5378(4)	0.4537(4)	0.1511(4)	0.013(1)
O6	16*f*	1.0	2O	0.5375(4)	0.5456(4)	0.3494(4)	0.016(1)
			$I\bar{4}2d$ model				
*X*1	8*d*	1.0	1Ca	¼	0.3755(2)	3/8	0.0106(6)
*X*2	8*d*	1.0	1Ca	¼	0.8748(2)	3/8	0.0124(7)
*X*3	8*c*	1.0	1Ca	½	0	0.5006(3)	0.0115(3)
*Y*1	16*e*	1.0	1.81Al + 0.19Fe	0.4995(3)	0.7502(3)	0.3747(3)	0.0102(4)
*Z*1	4*a*	0.93(2)	0.47Si + 0.03□	½	½	½	0.009(1)
*Z*2	8*d*	0.92(1)	0.92Si + 0.08□	¼	0.6244(3)	3/8	0.009(1)
*Z*3	4*b*	0.84(2)	0.42Si + 0.08□	½	0	¼	0.006(1)
*Z*4	8*d*	0.80(1)	0.80Si + 0.20□	¾	0.8741(3)	0.375000	0.005(1)
O1	16*f*	1.0	2O	0.5463(5)	0.5980(4)	0.4125(5)	0.010(1)
O2	16*f*	1.0	2O	0.2968(5)	0.5391(5)	0.2765(6)	0.016(1)
O3	16*f*	1.0	2O	0.3501(5)	0.7123(5)	0.4203(6)	0.013(1)

O4	16*f*	1.0	2O	0.4542(5)	0.8998(5)	0.3364(6)	0.018(1)
O5	16*f*	1.0	2O	0.7040(5)	0.9635(5)	0.4751(5)	0.012(1)
O6	16*f*	1.0	2O	0.6511(5)	0.7878(5)	0.3285(7)	0.015(1)

Table S2. Selected interatomic distances (Å) for $(H_4O_4)^{4-}$ substituted grossular from Wiluy River, Yakutia, Russia.

		$Ia\bar{3}d$ model			
*X*1–O1	2.494(1)	×4	*Z*1–O1	1.671(1)	×4
*X*1–O1	2.341(1)	×4			
<*X*1–O>	2.418		*Y*1–O1	1.936(1)	×4
		$I4_1/acd$ model			
*X*1–O1	2.345(2)	×4	*Y*1–O1	1.938(2)	×2
*X*1–O3	2.494(2)	×4	*Y*1–O2	1.934(2)	×2
<*X*1–O>	2.420		*Y*1–O3	1.938(2)	×2
			<*Y*1–O>	1.937	
*X*2–O2	2.343(2)	×4			
*X*2–O3	2.497(2)	×4	*Z*1–O2	1.674(2)	×2
<*X*2–O>	2.420		*Z*1–O3	1.672(2)	×2
			<Z1–O>	1.673	
*Z*2–O1	1.666(2)	×4			
		$I4_1/a$ model			
*X*1–O1	2.332(5)	×2	*Y*1–O6	1.933(4)	×2
*X*1–O5	2.492(4)	×2	<*Y*1–O>	1.941	
*X*1–O6	2.501(5)	×2			
*X*1–O2	2.356(5)	×2	*Y*2–O3	1.908(5)	×2
<*X*1–O>	2.420		*Y*2–O5	1.941(4)	×2
			*Y*2–O2	1.944(4)	×2
*X*2–O1	2.520(4)		<*Y*2–O>	1.931	
*X*2–O3	2.496(5)				
*X*2–O3	2.333(5)		*Z*1–O1	1.662(4)	×4
*X*2–O5	2.340(5)				
*X*2–O4	2.356(5)		*Z*2–O2	1.672(4)	×4
*X*2–O4	2.491(5)				
*X*2–O6	2.337(5)		*Z*3–O3	1.707(5)	
*X*2–O2	2.475(5)		*Z*3–O5	1.674(4)	
<*X*2–O>	2.419		*Z*3–O4	1.641(5)	
			*Z*3–O6	1.668(5)	
*Y*1–O1	1.931(4)	×2	<*Z*3–O>	1.673	
*Y*1–O4	1.960(5)	×2			
		$I\bar{4}2d$ model			
*X*1–O1	2.495(6)	×2	*Y*1–O1	1.972(7)	
*X*1–O2	2.330(7)	×2	*Y*1–O2	1.935(7)	
*X*1–O6	2.342(6)	×2	*Y*1–O6	1.951(6)	
*X*1–O3	2.484(7)	×2	*Y*1–O3	1.914(7)	
<*X*1–O>	2.413		*Y*1–O5	1.939(7)	
			*Y*1–O4	1.902(6)	
*X*2–O6	2.501(6)	×2	<*Y*1–O>	1.936	
*X*2–O3	2.341(6)	×2			
*X*2–O5	2.345(6)	×2	*Z*1–O1	1.648(6)	×4
*X*2–O4	2.500(6)	×2			
<*X*2–O>	2.421		*Z*2–O3	1.697(7)	×2
			*Z*2–O2	1.675(7)	×2
*X*3–O1	2.347(7)	×2	<*Z*2–O>	1.686	

*X*3–O2	2.495(6)	×2			
*X*3–O5	2.500(6)	×2	*Z*3–O4	1.684(5)	×4
*X*3–O4	2.351(6)	×2			
<*X*3–O>	2.423		*Z*4–O6	1.657(6)	×2
			*Z*4–O5	1.667(6)	×2
			<Z4–O>	1.662	

Table S3. Anisotropic displacement parameters (Å^2×10^3) for $(H_4O_4)^{4-}$ substituted grossular from Wiluy River, Yakutia, Russia. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

$Ia\bar{3}d$ model						
Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
*X*1	11.1(3)	11.1(3)	8.5(4)	0	0	-2.8(2)
*Y*1	9.3(4)	9.3(4)	9.3(4)	-1.0(2)	1.0(2)	1.0(2)
*Z*1	6.7(5)	6.7(5)	6.1(6)	0	0	0
O1	12.0(6)	10.8(6)	14.6(6)	-2.3(5)	-1.4(4)	0.6(5)
$I4_1/acd$ model						
*X*1	10.1(3)	10.1(3)	12.0(5)	0	0	2.7(4)
*X*2	10.1(4)	7.7(4)	14.4(4)	0	-2.7(2)	0
*Y*1	6.9(6)	8.5(7)	12.3(6)	-1.0(3)	-1.3(3)	-0.8(4)
*Z*1	5.6(6)	5.0(6)	9.7(6)	0	-0.4(4)	0
*Z*2	5.9(6)	5.9(6)	9.0(8)	0	0	0
O1	11.1(9)	9.5(9)	17.8(9)	-2.5(7)	0.5(7)	-0.3(8)
O2	9.5(9)	14.6(9)	15.8(9)	1.3(7)	-1.1(7)	-2.4(8)
O3	10.2(9)	13.0(9)	16.1(9)	2.6(7)	0.3(7)	2.2(7)
$I4_1/a$ model						
*X*1	9.5(11)	11.3(11)	14.1(5)	0	0	-2.7(3)
*X*2	8.5(4)	10.5(4)	15.7(4)	-2.5(2)	0.0(8)	2.3(8)
*Y*1	4.3(15)	10.2(16)	7.8(13)	3.9(11)	-3.1(11)	1.1(9)
*Y*2	6.3(15)	12.0(16)	19.0(14)	0.0(12)	-1.3(11)	0.4(9)
*Z*1	6.1(14)	6.1(14)	12.2(18)	0	0	0
*Z*2	4.9(13)	4.9(13)	8.4(17)	0	0	0
*Z*3	5.9(5)	6.1(5)	10.6(6)	-0.5(3)	-0.6(13)	-2.5(12)
O1	11(3)	6(3)	29(2)	1(2)	-8(2)	4(2)
O2	16(3)	14(2)	12.5(19)	8(2)	4(2)	-2(2)
O3	15(3)	15(3)	17(2)	-5(2)	-4(2)	-2(2)
O4	16(3)	5(2)	18(2)	1(2)	0(2)	-7(2)
O5	9(3)	9(3)	22(2)	-5(2)	-2(2)	0(2)
O6	19(3)	14(3)	15(2)	6(2)	-7(2)	-3(3)
$I\bar{4}2d$ model						
*X*1	8.8(13)	9.3(12)	18.0(13)	0	4.8(10)	0
*X*2	12.4(14)	8.0(12)	13.6(11)	0	-0.6(10)	0
*X*3	15.9(14)	5.8(13)	14.6(7)	0	0	-2.7(5)
*Y*1	7.8(9)	8.5(9)	13.4(8)	-1.2(4)	1.6(4)	0.8(4)
*Z*1	7.4(17)	7.4(17)	12(2)	0	0	0
*Z*2	7.5(19)	7.7(18)	16.7(18)	0	0.4(12)	0
*Z*3	4.2(19)	4.2(19)	10(3)	0	0	0
*Z*4	4.7(16)	4.2(16)	5.1(15)	0	0.5(10)	0
O1	10(3)	6(3)	39(4)	-11(3)	3(4)	1(3)

$Ia\bar{3}d$ model						
Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	12(3)	21(3)	18(3)	7(3)	-3(3)	-1(3)
O3	14(3)	22(3)	16(3)	6(3)	-3(3)	8(3)
O4	14(3)	15(3)	6(2)	6(2)	-3(3)	0(3)
O5	11(3)	7(3)	20(3)	-2(3)	2(3)	-4(3)
O6	7(3)	11(3)	18(3)	-3(3)	6(3)	-3(3)