Supplementary materials

Table *S*1 Structural parameters for $Ga_2O_3(ZnO)_6$ in a non-conventional setting.

	x_1^0	x_2^0	x_3^0	x_4^0	Δ	V_{x2}
subsystem 1						
*M*1	0	0.38428(2)	0	0	7/16	-21/16
*M*1a	0	0.89015(19)	0.098(10)	0.7560(7)	1/16	
*M*1b	1/2	0.86484(11)	0	3/4	1/16	
*M*1c	0	0.87414(6)	0	1/4	1/16	
subsystem 2						
O1	0	0.88496(9)	1/2	0	1/2	-27/16

$V_{x1}=V_{x3}=0$ for *M*1 and O1.

Occupation factors are 0.236(2) for *M*1a, 0.528(4) for *M*1b, and 1 for others.

The crenel function is used for occupation of *M*1a, *M*1b, and *M*1c.

For *M*1 and O1, the modulation function for fractional coordinates *u* consists of a zigzag function and an additional deviation expressed in terms of the Fourier series, which are the same to those in Table S1.

For *M*1 and O1, the modulation function for fractional coordinates *u* consists of two terms;

$u=u_z+u_h$.

The first term is a zigzag function defined by

$$u_z=\begin{cases}(2V_{x_j}/\Delta)(\bar{x}_4-x_4^0) & (x_4^0-\Delta/2\le\bar{x}_4\le x_4^0+\Delta/2)\\ (-2V_{x_j}/\Delta)(\bar{x}_4-x_4^0-1/2) & (x_4^0+1/2-\Delta/2\le\bar{x}_4\le x_4^0+1/2+\Delta/2)\end{cases},$$

where $\bar{x}_4$ is a phase parameter, or the 4th coordinate of an occupation domain in a basic (that is, V_{xj} is assumed to 0) structure. (see Fig. *S*1)

The second term is an additional deviation expressed in terms of the Fourier series;

$$u_h=\sum_{n>0}[A_n sin(2\pi n\bar{x}_4)+B_n\cos(2\pi n\bar{x}_4)]\cdot$$

Table *S*1 Structural parameters for $Ga_2O_3(ZnO)_6$ in a non-conventional setting. (*cont*. 1)

		x_2		x_3	
		A_n	B_n	A_n	B_n
1st substructure					
*M*1	*n*=1	0	-0.00341(3)	0.1058(3)	0
	2	0.00160(5)	0	0	-0.0490(3)
	3	0	0.00208(3)	0.0015(3)	0
	4	0.00002(5)	0	0	0.0204(3)
	5	0	-0.00024(3)	-0.0210(3)	0
	6	0.00133(5)	0	0	-0.0005(4)
	7	0	0	-0.0129(4)	0
2nd substructure					
O1	*n*=1	0	0.01150(11)	0.093(2)	0
	2	0.00037(12)	0	0	-0.1091(19)
	3	0	0.00525(13)	-0.070(2)	0
	4	0.00030(13)	0	0	0.004(2)
	5	0	-0.00151(13)	-0.037(2)	0
	6	0.00101(13)	0	0	-0.013(2)
	7	0	0.00094(14)	0.015(2)	0
	8	-0.00071(15)	0	0	0.012(3)
	9	0	-0.00061(11)	0	0

A_n=B_n=0 for x_1 at all sites.

Table *S*1 Structural parameters for $Ga_2O_3(ZnO)_6$ in a non-conventional setting. (*cont*. 2)

		U_{11}	U_{22}	U_{33}	U_{23}
1st substructure					
*M*1		0.00950(19)	0.00838(16)	0.01504(19)	0
	A_1	0	0	0	-0.00540(10)
	B_1	-0.0012(2)	0.0004(2)	0.0032(2)	0
	A_2	-0.0008(4)	-0.0010(3)	0.0048(4)	0
	B_2	0	0	0	-0.00097(13)
	A_3	0	0	0	0.00097(14)
	B_3	0.0020(2)	-0.0004(2)	0.0049(3)	0
	A_4	-0.0011(4)	0.0003(3)	-0.0066(4)	0
	B_4	0	0	0	0.00049(15)
	A_5	0	0	0	0.00080(16)
	B_5	-0.0008(2)	0.0003(2)	-0.0023(3)	0
	A_6	0.0000(3)	-0.0005(3)	0.0021(4)	0
	B_6	0	0	0	-0.00035(16)
	A_7	0	0	0	-0.00037(19)
	B_7	0	0	0	0
*M*1a		0.068(3)	0.0092(13)	0.024(7)	-0.004(2)
*M*1b		0.0178(12)	0.0078(9)	0.0083(9)	0
*M*1c		0.0084(5)	0.0076(5)	0.0107(5)	0

The anisotropic thermal parameter is given in terms of the Fourier series including zeroth order term;

$$U_{\alpha\beta} = U^0_{\alpha\beta} + \sum_{n>0}[A_n sin(2\pi n \bar{x}_4) + B_n \cos(2\pi n \bar{x}_4)] \cdot$$

$U^0_{12} = U^0_{13} = 0$ at all sites.

A_n=B_n=0 for U_{12} and U_{13} at *M*1.

Table *S*1 Structural parameters for $Ga_2O_3(ZnO)_6$ in a non-conventional setting. (*cont*. 3)

		U_{11}	U_{22}	U_{33}	U_{23}
2nd substructure					
O1		0.0228(9)	0.0139(7)	0.0247(10)	0
	A_1	0	0	0	-0.0121(11)
	B_1	0.0211(15)	0.0002(9)	0.0047(12)	0
	A_2	-0.0155(13)	0.0032(10)	0.0134(14)	0
	B_2	0	0	0	-0.0014(9)
	A_3	0	0	0	-0.0064(10)
	B_3	-0.0128(12)	-0.0014(10)	-0.0037(13)	0
	A_4	0.0047(10)	0.0020(10)	0.0092(13)	0
	B_4	0	0	0	-0.0011(10)
	A_5	0	0	0	-0.0033(11)
	B_5	-0.0031(11)	-0.0004(12)	-0.0022(13)	0
	A_6	0.0083(15)	-0.0017(11)	0.0047(14)	0
	B_6	0	0	0	0.0028(11)
	A_7	0	0	0	0.0013(10)
	B_7	0.0148(16)	-0.0034(12)	-0.0019(17)	0
	A_8	-0.017(2)	0.0011(12)	-0.0026(15)	0
	B_8	0	0	0	0.0043(13)
	A_9	0	0	0	0
	B_9	-0.0084(11)	-0.0024(10)	-0.0040(10)	0

$U_{12}^0 = U_{13}^0 = 0$ and $A_n = B_n = 0$ for U_{12} and U_{13}.

Table *S*2 Structural parameters for $Ga_2O_3(ZnO)_9$ in a non-conventional setting.

	x_1^0	x_2^0	x_3^0	x_4^0	Δ	V_{x2}
subsystem 1						
*M*1	0	0.38457(2)	0	0	5/11	-15/8
*M*1a	0	0.45841(19)	0	3/4	1/22	
*M*1b	1/2	0.43144(18)	0	3/4	1/22	
*M*1c	0	-0.69258(8)	0	1/4	1/22	
subsystem 2						
O1	0	0.88483(9)	1/2	0	1/2	-9/4

$V_{x1}=V_{x3}=0$ at *M*1 and O1.

Occupation factors are 0.557(4) for *M*1a, 0.443(4) for *M*1b, and 1 for others.

The crenel function is used for occupation of *M*1a, M1b, and *M*1c.

For *M*1 and O1, the modulation function for fractional coordinates *u* consists of a zigzag function and an additional deviation expressed in terms of the Fourier series, which are the same to those in Table *S*1.

Table *S*2 Structural parameters for $Ga_2O_3(ZnO)_9$ in a non-conventional setting. (*cont*. 1)

		x_2		x_3	
		A_n	B_n	A_n	B_n
1st substructure					
*M*1	*n*=1	0	-0.00613(4)	0.1031(2)	0
	2	0.00107(4)	0	0	-0.0515(2)
	3	0	0.00363(4)	-0.0328(3)	0
	4	-0.00051(4)	0	0	0.0242(2)
	5	0	-0.00041(4)	-0.0140(3)	0
	6	0.00003(4)	0	0	-0.0151(3)
	7	0	0.00027(4)	0.0161(3)	0
	8	-0.00107(4)	0	0	0.0011(3)
	9	0	0.00002(4)	0.0111(3)	0
	10	0	0	0	-0.0014(3)
2nd substructure					
O1	*n*=1	0	0.00974(11)	0.1024(19)	0
	2	0.00007(13)	0	0	-0.1190(16)
	3	0	0.00743(12)	-0.0408(17)	0
	4	-0.00036(12)	0	0	-0.0245(16)
	5	0	-0.00068(13)	0.0362(18)	0
	6	0.00000(14)	0	0	-0.0167(17)
	7	0	0.00118(14)	0.0202(19)	0
	8	-0.00035(14)	0	0	0.0048(19)
	9	0	-0.00069(15)	-0.008(2)	0
	10	0.00014(15)	0	0	-0.007(2)
	11	0	0.00106(16)	0.014(2)	0
	12	-0.00063(11)	0	0	0

A_n=B_n=0 for x_1 at all sites.

Table *S*2 Structural parameters for $Ga_2O_3(ZnO)_9$ in a non-conventional setting. (*cont*. 2)

		U_{11}	U_{22}	U_{33}	U_{23}
1st substructure					
*M*1		0.00815(15)	0.01005(19)	0.01727(16)	0
	A_1	0	0	0	-0.00488(12)
	B_1	-0.0004(2)	-0.0002(5)	-0.0010(4)	0
	A_2	-0.0013(2)	-0.0003(3)	0.0036(2)	0
	B_2	0	0	0	-0.00050(15)
	A_3	0	0	0	0.00082(14)
	B_3	0.0009(2)	-0.0001(5)	0.0011(4)	0
	A_4	-0.0010(2)	0.0001(3)	-0.0039(3)	0
	B_4	0	0	0	0.00085(15)
	A_5	0	0	0	0.00050(14)
	B_5	-0.0014(2)	0.0002(5)	-0.0050(4)	0
	A_6	0.0010(3)	-0.0004(3)	0.0026(3)	0
	B_6	0	0	0	-0.00038(16)
	A_7	0	0	0	-0.00016(18)
	B_7	0.0012(3)	0.0000(5)	0.0034(4)	0
	A_8	-0.0002(2)	0.0005(3)	-0.0022(3)	0
	B_8	0	0	0	-0.00023(17)
	A_9	0	0	0	0.00028(19)
	B_9	0.0000(2)	0.0000(5)	-0.0018(4)	0
	A_{10}	0	0	0	0
	B_{10}	0	0	0	0.0006(2)
*M*1a		0.076(3)	0.0118(17)	0.0391(19)	0
*M*1b		0.0270(16)	0.0081(16)	0.0113(14)	0
*M*1c		0.0086(5)	0.0088(7)	0.0136(6)	0

The anisotropic thermal parameter is given as in Table *S*1.

$U_{12}^0 = U_{13}^0 = 0$ at all sites.

A_n=B_n=0 for U_{12} and U_{13} at *M*1.

Table *S*2 Structural parameters for $Ga_2O_3(ZnO)_9$ in a non-conventional setting. (*cont*. 3)

		U_{11}	U_{22}	U_{33}	U_{23}
2nd substructure					
O1		0.0175(8)	0.0146(8)	0.0264(8)	0
	A_1	0	0	0	-0.0130(11)
	B_1	0.0155(12)	0.0008(11)	0.0028(11)	0
	A_2	-0.0138(11)	0.0035(13)	0.0129(12)	0
	B_2	0	0	0	0.0012(10)
	A_3	0	0	0	-0.0081(10)
	B_3	-0.0110(11)	-0.0011(12)	-0.0044(12)	0
	A_4	0.0075(10)	0.0037(13)	0.0089(11)	0
	B_4	0	0	0	0.0031(10)
	A_5	0	0	0	-0.0052(10)
	B_5	0.0054(10)	-0.0003(14)	0.0002(11)	0
	A_6	-0.0016(10)	0.0023(13)	0.0030(13)	0
	B_6	0	0	0	-0.0014(11)
	A_7	0	0	0	-0.0023(11)
	B_7	0.0000(10)	-0.0011(15)	0.0004(12)	0
	A_8	-0.0057(12)	0.0014(14)	0.0003(13)	0
	B_8	0	0	0	0.0010(11)
	A_9	0	0	0	-0.0003(12)
	B_9	-0.0095(12)	0.0009(15)	-0.0027(13)	0
	A_{10}	0.0101(14)	-0.0013(15)	0.0054(19)	0
	B_{10}	0	0	0	0.0000(12)
	A_{11}	0	0	0	0.0017(12)
	B_{11}	0.0121(13)	-0.0000(17)	0.0019(13)	0
	A_{12}	-0.0066(10)	0.0012(10)	-0.0013(11)	0
	B_{12}	0	0	0	0

$U^0_{12}=U^0_{13}=0$, and $A_n=B_n=0$ for U_{12} and U_{13}.

Table *S*3 Structural parameters for $Ga_2O_3(ZnO)_6$ in a conventional setting.

	x_1^0	x_2^0	x_3^0	x_4^0	Δ	V_{x2}
subsystem 1						
*M*1	0	0.38426(4)	0	0	3/8	3/8
*M*1a	0	-0.10985(19)	0.049(5)	0.804(6)	1/8	
*M*1b	1/2	-0.13516(11)	0	3/4	1/8	
*M*1c	0	0.87414(6)	0	1/4	1/8	
*M*2	0	0.88428(2)	1/2	1/2	1/2	1/2
subsystem 2						
O1	0	0.63435(13)	1/4	3/4	1/2	9/16
O2	0	0.13556(14)	3/4	1/4	1/2	9/16

$V_{x1}=V_{x3}=0$ for *M*1, *M*2, O1, and O2.

Occupation factors are 0.236(2) for *M*1a, 0.528(4) for *M*1b, and 1 for others.

The crenel function is used for occupation of *M*1a, *M*1b, and *M*1c.

For *M*1, *M*2, O1, and O2, the modulation function for fractional coordinates *u* consists of a zigzag function and an additional deviation expressed in terms of the Fourier series, which are the same to those in Table *S*1.

Table *S*3 Structural parameters for $Ga_2O_3(ZnO)_6$ in a conventional setting. (*cont*. 1)

		x_2		x_3	
		A_n	B_n	A_n	B_n
1st substructure					
*M*1	*n*=1	0	-0.00109(4)	0.0464(2)	0
	2	0.00297(5)	0	0	-0.0243(3)
	3	0	0	-0.0097(2)	0
*M*2	*n*=1	0	0.00341(3)	-0.0594(2)	0
	2	0.00027(3)	0	0	-0.0247(2)
	3	0	-0.00184(3)	-0.0113(2)	0
	4	0	0	0	0.01023(15)
2nd substructure					
O1	*n*=1	0.01080(17)	0	0	0.0523(16)
	2	-0.00131(18)	0	0	-0.0468(14)
	3	-0.00626(17)	0	0	0.0416(15)
	4	-0.00121(18)	0	0	0.0167(14)
O2	*n*=1	-0.0122(2)	0	0	-0.0407(19)
	2	0.00057(19)	0	0	-0.0623(15)
	3	0.00424(18)	0	0	-0.0284(18)
	4	0.00182(19)	0	0	-0.0205(16)

A_n=B_n=0 for x_1 at all sites.

Table *S*3 Structural parameters for $Ga_2O_3(ZnO)_6$ in a conventional setting. (*cont*. 2)

		U_{11}	U_{22}	U_{33}	U_{23}
1st substructure					
*M*1		0.0106(3)	0.0081(2)	0.0216(3)	0
	A_1	0	0	0	-0.0058(2)
	B_1	0.0015(3)	-0.0002(3)	0.0105(5)	0
	A_2	-0.0031(4)	-0.0008(4)	-0.0063(5)	0
	B_2	0	0	0	-0.0006(2)
	A_3	0	0	0	0.0018(2)
	B_3	0	0	0	0
*M*1a		0.068(3)	0.0092(13)	0.024(7)	-0.004(2)
*M*1b		0.0178(12)	0.0078(9)	0.0083(9)	0
*M*1c		0.0084(5)	0.0076(5)	0.0107(5)	0
*M*2		0.00950(19)	0.00838(16)	0.01504(19)	0
	A_1	0	0	0	0.0050(2)
	B_1	0.0012(2)	-0.0004(2)	-0.0032(3)	0
	A_2	-0.0008(3)	-0.0005(2)	0.0027(2)	0
	B_2	0	0	0	-0.0013(2)
	A_3	0	0	0	-0.0002(2)
	B_3	-0.0012(2)	0.0002(2)	-0.0027(3)	0
	A_4	0	0	0	0
	B_4	0	0	0	0.00049(15)

The anisotropic thermal parameter is given as in Table *S*1.

$U_{12}^0 = U_{13}^0 = 0$ at all sites.

$A_n = B_n = 0$ for U_{12} and U_{13} at *M*1 and *M*2.

Table *S*3 Structural parameters for $Ga_2O_3(ZnO)_6$ in a conventional setting. (*cont*. 3)

		U_{11}	U_{22}	U_{33}	U_{23}
2nd substructure					
O1		0.0143(9)	0.0115(11)	0.0207(12)	0
	A_1	0.0043(17)	0.0013(14)	0.0021(18)	0
	B_1	0	0	0	-0.0078(15)
	A_2	0.0007(13)	0.0002(14)	-0.0116(19)	0
	B_2	0	0	0	-0.0002(12)
	A_3	0.0045(17)	0.0031(14)	-0.0010(19)	0
	B_3	0	0	0	0.0036(13)
	A_4	0.0016(15)	0.0016(14)	0.0070(16)	0
	B_4	0	0	0	0.0044(13)
O2		0.0312(17)	0.0163(13)	0.0287(16)	0
	A_1	-0.038(3)	0.0009(15)	-0.007(2)	0
	B_1	0	0	0	0.0164(19)
	A_2	0.030(3)	-0.0066(18)	-0.015(3)	0
	B_2	0	0	0	-0.0027(15)
	A_3	-0.021(2)	0.0003(15)	-0.008(2)	0
	B_3	0	0	0	-0.0092(18)
	A_4	0.0079(16)	0.0023(16)	0.011(2)	0
	B_4	0	0	0	-0.0023(17)

$U_{12}^0 = U_{13}^0 = 0$ at all sites.

A_n=B_n=0 for U_{12} and U_{13} at all sites.

Table *S*4 Structural parameters for $Ga_2O_3(ZnO)_9$ in a conventional setting.

	x_1^0	x_2^0	x_3^0	x_4^0	Δ	V_{x2}
subsystem 1						
*M*1	0	0.63438(3)	1/4	3/4	9/22	-99/176
*M*1a	0	-0.04159(19)	1/4	0	1/11	
*M*1b	1/2	-0.06856(18)	1/4	0	1/11	
*M*2	0	0.13443(2)	3/4	1/4	1/2	-11/16
subsystem 2						
O1	0	0.38420(13)	0	0	1/2	-3/4
O2	0	0.88545(15)	1/2	1/2	1/2	-3/4

$V_{x1}=V_{x3}=0$ at *M*1, *M*2, O1, and O2.

Occupation factors are 0.557(4) for *M*1a, 0.443(4) for *M*1b, and 1 for others.

The crenel function is used for occupation of *M*1a and *M*1b.

For *M*1, *M*2, O1, and O2, the modulation function for fractional coordinates *u* consists of a zigzag function and an additional deviation expressed in terms of the Fourier series, which are the same to those in Table *S*1.

Table *S*4 Structural parameters for $Ga_2O_3(ZnO)_9$ in a conventional setting. (*cont*. 1)

		x_2		x_3	
		A_n	B_n	A_n	B_n
1st substructure					
*M*1	*n*=1	0.00576(4)	0	0	0.0509(2)
	2	-0.00146(4)	0	0	0.02017(18)
	3	0.00219(4)	0	0	0.0158(2)
	4	-0.00062(5)	0	0	0.02014(18)
	5	0	0	0	-0.01453(18)
*M*2	*n*=1	-0.00641(3)	0	0	-0.0522(2)
	2	-0.00133(3)	0	0	0.03131(18)
	3	-0.00498(3)	0	0	-0.0169(2)
	4	-0.00106(4)	0	0	0.00403(17)
	5	-0.00072(4)	0	0	-0.0006(2)
2nd substructure					
O1	*n*=1	0	-0.00868(19)	0.0582(14)	0
	2	0.00021(19)	0	0	0.0562(13)
	3	0	-0.00812(18)	-0.0243(13)	0
	4	-0.00071(18)	0	0	0.0146(12)
	5	0	0.00187(19)	0.0282(14)	0
	6	0.00000(14)	0	0	0
O2	*n*=1	0	0.0108(2)	-0.0443(14)	0
	2	-0.0001(2)	0	0	0.0628(14)
	3	0	0.00675(19)	0.0165(14)	0
	4	-0.00002(19)	0	0	0.0098(13)
	5	0	0.00051(19)	-0.0080(13)	0
	6	0	0	0	0.0084(8)

A_n=B_n=0 for x_1 at all sites.

Table *S*4 Structural parameters for $Ga_2O_3(ZnO)_9$ in a conventional setting. (*cont*. 2)

		U_{11}	U_{22}	U_{33}	U_{23}
1st substructure					
*M*1		0.00793(18)	0.0099(3)	0.0161(2)	0
	A_1	0.0000(3)	-0.0001(5)	-0.0014(3)	0
	B_1	0	0	0	-0.0043(2)
	A_2	0.0009(3)	0.0001(4)	-0.0042(4)	0
	B_2	0	0	0	0.0002(2)
	A_3	0.0002(3)	0.0002(4)	-0.0034(3)	0
	B_3	0	0	0	-0.0006(2)
	A_4	-0.0002(3)	-0.0002(5)	-0.0029(4)	0
	B_4	0	0	0	0.0007(2)
	A_5	0	0	0	0
	B_5	0	0	0	0.0001(2)
*M*1a		0.076(3)	0.0118(17)	0.0391(19)	0
*M*1b		0.0270(16)	0.0081(16)	0.0113(14)	0
*M*2		0.00863(16)	0.0098(3)	0.0192(2)	0
	A_1	0.0005(2)	-0.0006(3)	0.0028(3)	0
	B_1	0	0	0	0.0055(2)
	A_2	0.0023(2)	-0.0002(3)	-0.0016(2)	0
	B_2	0	0	0	0.0008(2)
	A_3	-0.0002(2)	0.0001(3)	0.0005(3)	0
	B_3	0	0	0	0.0010(2)
	A_4	-0.0012(2)	-0.0004(3)	-0.0035(2)	0
	B_4	0	0	0	0.0010(2)
	A_5	-0.0015(2)	0.0001(3)	-0.0038(3)	0
	B_5	0	0	0	-0.0009(2)

The anisotropic thermal parameter is given as in Table *S*1.

$U_{12}^0 = U_{13}^0 = 0$ at all sites.

$A_n = B_n = 0$ for U_{12} and U_{13} at *M*1 and *M*2.

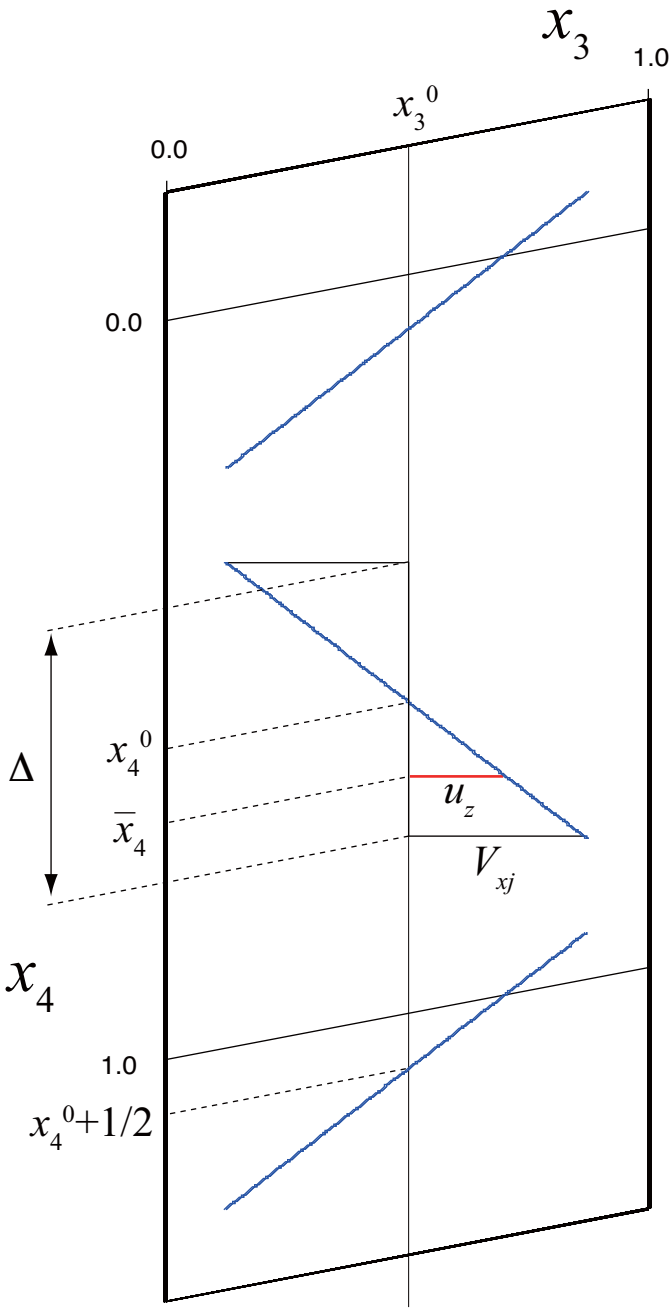
Table *S*4 Structural parameters for $Ga_2O_3(ZnO)_9$ in a conventional setting. (*cont*. 3)

		U_{11}	U_{22}	U_{33}	U_{23}
2nd substructure					
O1		0.0109(10)	0.0158(14)	0.0251(13)	0
	A_1	0	0	0	-0.0113(16)
	B_1	-0.0034(13)	-0.001(2)	-0.0009(16)	0
	A_2	-0.0037(13)	0.002(2)	0.018(2)	0
	B_2	0	0	0	-0.0012(15)
	A_3	0	0	0	-0.0084(16)
	B_3	0.0014(15)	0.0020(19)	0.0017(16)	0
	A_4	0.0018(15)	0.005(2)	0.0092(19)	0
	B_4	0	0	0	-0.0021(13)
	A_5	0	0	0	-0.0075(16)
	B_5	-0.0054(15)	-0.001(2)	0.0001(14)	0
	A_6	-0.0016(10)	0.0023(13)	0.0030(13)	0
	B_6	0	0	0	0
O2		0.0241(14)	0.0134(13)	0.0276(14)	0
	A_1	0	0	0	0.0147(16)
	B_1	0.028(2)	0.001(2)	0.0048(18)	0
	A_2	-0.024(2)	0.005(2)	0.007(2)	0
	B_2	0	0	0	-0.0012(16)
	A_3	0	0	0	0.0078(15)
	B_3	-0.0205(18)	0.000(2)	-0.0070(19)	0
	A_4	0.0132(17)	0.0023(18)	0.0086(16)	0
	B_4	0	0	0	-0.0041(15)
	A_5	0	0	0	0.0029(14)
	B_5	0.0054(14)	-0.001(2)	0.0006(18)	0
	A_6	0	0	0	0
	B_6	0	0	0	0.0014(11)

$U_{12}^0 = U_{13}^0 = 0$ at all sites.

$A_n = B_n = 0$ for U_{12} and U_{13} at all sites.

Figure S1 Zigzag function



$$u_z = \begin{cases} (2V_{x_j}/\Delta)(\bar{x}_4 - x_4^0) & (x_4^0 - \Delta/2 \le \bar{x}_4 \le x_4^0 + \Delta/2) \\ (-2V_{x_j}/\Delta)(\bar{x}_4 - x_4^0 - 1/2) & (x_4^0 + 1/2 - \Delta/2 \le \bar{x}_4 \le x_4^0 + 1/2 + \Delta/2) \end{cases}$$