Supplementary data

The tables of data shown below are not normally printed in *Acta Cryst. Section C* but the data will be available electronically *via* the online contents pages at

http://journals.iucr.org/c/journalhomepage.html

Table *S*1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for sample–I*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	x	y	z	$U_{\rm eq}$
K1	0.303 (3)	0	0	0.234 (3)	0.089 (6)
Ga1	0.9326 (14)	**0.118144** (10)	**0.162373** (10)	0.5	0.00472 (4)
Al1	0.0640 (16)	**0.118144**	**0.162373**	0.5	0.00472
Ga2	0.756 (5)	**0.203530** (11)	**0.310781** (11)	0	0.00525 (5)
Al2	0.077 (14)	**0.203530**	**0.310781**	0	0.00525
Ti2	0.166 (13)	**0.203530**	**0.310781**	0	0.00525
Ti3	0.730 (13)	**0.221445** (15)	**0.035922** (14)	0	0.00593 (6)
Ga3	0.202 (6)	**0.221445**	**0.035922**	0	0.00593
Al3	0.069 (14)	**0.221445**	**0.035922**	0	0.00593
Ti4	0.964 (2)	**0.119442** (18)	**0.542960** (17)	0	0.00905 (6)
Ga4	0.036 (2)	**0.119442**	**0.542960**	0	0.00905
Ga5	0.0034 (8)	0.057 (3)	0.100 (3)	0.5	0.01
O1	1	0.40977 (7)	0.02065 (6)	0	0.0059 (2)
O2	1	0.39445 (6)	0.15152 (6)	0.5	0.0057 (2)
O3	1	0.28044 (6)	0.00190 (7)	0.5	0.0063 (2)
O4	1	0.26450 (7)	0.13104 (6)	0	0.0061 (2)
O5	1	0.18949 (6)	0.23637 (6)	0.5	0.0053 (2)
O6	1	0.15538 (6)	0.06769 (6)	0.5	0.0062 (2)
O7	1	0.06143 (6)	0.16830 (7)	0	0.0070 (2)

Table *S*2. *Anisotropic displacement parameters* (Å^2) *for sample–I*

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.052 (2)	0.052 (2)	0.163 (19)	0	0	0
Ga1	0.00498 (7)	0.00556 (7)	0.00361 (7)	−0.00019 (5)	0	0
Ga2	0.00549 (8)	0.00657 (8)	0.00370 (8)	0.00028 (5)	0	0
Ti3	0.00858 (10)	0.00475 (9)	0.00446 (10)	0.00003 (7)	0	0
Ti4	0.01043 (11)	0.00974 (11)	0.00697 (11)	−0.00056 (8)	0	0
O1	0.0081 (4)	0.0042 (3)	0.0054 (4)	−0.0015 (3)	0	0
O2	0.0058 (4)	0.0066 (4)	0.0046 (4)	0.0006 (3)	0	0
O3	0.0050 (4)	0.0079 (4)	0.0060 (4)	0.0026 (3)	0	0
O4	0.0088 (4)	0.0048 (3)	0.0048 (4)	−0.0013 (3)	0	0
O5	0.0062 (4)	0.0051 (3)	0.0045 (4)	−0.0004 (3)	0	0
O6	0.0065 (4)	0.0072 (4)	0.0049 (4)	0.0024 (3)	0	0
O7	0.0055 (4)	0.0120 (4)	0.0035 (4)	0.0030 (3)	0	0

Table *S*3. *Geometric parameters (Å, °) for sample–I*

Ga1—O5	1.8602 (11)	Ti3—O6^{iv}	1.9993 (8)
Ga1—O6	1.8413 (12)	Ti3—O6	1.9993 (8)
Ga1—O7	1.8172 (7)	Ti3—O7^{v}	2.0072 (12)
Ga1—O7^{i}	1.8172 (7)	Ti4—O1^{iii}	1.9602 (7)
Ga2—O2^{ii}	1.8998 (12)	Ti4—O1^{ii}	1.9602 (7)
Ga2—O4^{iii}	1.9185 (7)	Ti4—O1^{vi}	1.9819 (11)
Ga2—O4^{ii}	1.9185 (7)	Ti4—O2^{vi}	1.9641 (8)
Ga2—O5^{iv}	2.0286 (8)	Ti4—O2^{vii}	1.9641 (8)
Ga2—O5	2.0286 (8)	Ti4—O3^{ii}	1.9855 (12)
Ga2—O5^{ii}	2.1158 (11)	Ga5—O6	1.88 (6)
Ti3—O3^{iv}	1.9381 (7)	Ga5—O6^{viii}	2.47 (6)
Ti3—O3	1.9381 (7)	Ga5—O7	1.95 (4)
Ti3—O4	1.8895 (12)	Ga5—O7^{i}	1.95 (4)

Symmetry codes: (i) $x, y, 1+z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, -\frac{1}{2}-z$; (iv) $x, y, z-1$; (v) $y, -x, -z$; (vi) $y, 1-x, -z$; (vii) $y, 1-x, 1-z$; (viii) $-y, x, z$.

Table *S*4. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for sample–II*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	x	y	z	$U_{\rm eq}$
K1	0.310 (4)	0	0	0.225 (6)	0.092 (11)
Ga1	0.8351 (15)	**0.117996** (11)	**0.162518** (11)	0.5	0.00521 (4)
Al1	0.1596 (17)	**0.117996**	**0.162518**	0.5	0.00521
Ga2	0.610 (6)	**0.203739** (12)	**0.310893** (12)	0	0.00607 (5)
Al2	0.167 (16)	**0.203739**	**0.310893**	0	0.00607
Ti2	0.223 (15)	**0.203739**	**0.310893**	0	0.00607
Ti3	0.659 (15)	**0.221305** (15)	**0.036084** (14)	0	0.00640 (6)
Ga3	0.178 (7)	**0.221305**	**0.036084**	0	0.00640
Al3	0.163 (16)	**0.221305**	**0.036084**	0	0.00640
Ti4	0.978 (3)	**0.119804** (17)	**0.542926** (17)	0	0.00966 (6)
Ga4	0.022 (3)	**0.119804**	**0.542926**	0	0.00966
Ga5	0.0053 (8)	0.062 (2)	0.104 (2)	0.5	0.01
O1	1	0.40946 (6)	0.02052 (6)	0	0.0064 (2)
O2	1	0.39415 (6)	0.15200 (6)	0.5	0.0065 (2)
O3	1	0.28021 (6)	0.00199 (6)	0.5	0.0068 (2)
O4	1	0.26458 (6)	0.13112 (6)	0	0.0070 (2)
O5	1	0.18948 (6)	0.23623 (6)	0.5	0.0066 (2)
O6	1	0.15515 (6)	0.06782 (6)	0.5	0.0070 (2)
O7	1	0.06154 (6)	0.16841 (7)	0	0.0081 (2)

Table *S*5. *Anisotropic displacement parameters* (Å^2) *for sample–II*

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.051 (2)	0.051 (2)	0.18 (3)	0	0	0
Ga1	0.00533 (7)	0.00602 (7)	0.00428 (7)	−0.00021 (5)	0	0
Ga2	0.00595 (9)	0.00739 (9)	0.00485 (9)	0.00022 (6)	0	0
Ti3	0.00853 (11)	0.00525 (10)	0.00542 (11)	0.00006 (7)	0	0
Ti4	0.01099 (11)	0.01015 (10)	0.00785 (11)	−0.00049 (7)	0	0
O1	0.0076 (3)	0.0055 (3)	0.0059 (4)	−0.0013 (3)	0	0
O2	0.0053 (3)	0.0077 (4)	0.0066 (4)	0.0013 (3)	0	0
O3	0.0058 (3)	0.0081 (4)	0.0063 (4)	0.0023 (3)	0	0
O4	0.0084 (4)	0.0056 (3)	0.0071 (4)	−0.0010 (3)	0	0
O5	0.0066 (3)	0.0055 (3)	0.0076 (4)	−0.0010 (3)	0	0
O6	0.0061 (3)	0.0078 (4)	0.0069 (4)	0.0016 (3)	0	0
O7	0.0064 (3)	0.0115 (4)	0.0063 (4)	0.0028 (3)	0	0

Table *S*6. *Geometric parameters (Å, °) for sample–II*

Ga1—O5	1.8545 (11)	Ti3—O6^{iv}	1.9955 (8)
Ga1—O6	1.8372 (12)	Ti3—O6	1.9955 (8)
Ga1—O7	1.8102 (7)	Ti3—O7^{v}	2.0053 (12)
Ga1—O7^{i}	1.8102 (7)	Ti4—O1^{iii}	1.9540 (7)
Ga2—O2^{ii}	1.8906 (11)	Ti4—O1^{ii}	1.9540 (7)
Ga2—O4^{iii}	1.9105 (7)	Ti4—O1^{vi}	1.9887 (11)
Ga2—O4^{ii}	1.9105 (7)	Ti4—O2^{vi}	1.9636 (7)
Ga2—O5^{iv}	2.0274 (7)	Ti4—O2^{vii}	1.9636 (7)
Ga2—O5	2.0274 (7)	Ti4—O3^{ii}	1.9796 (11)
Ga2—O5^{ii}	2.1081 (11)	Ga5—O6	1.80 (4)
Ti3—O3^{iv}	1.9332 (7)	Ga5—O6^{viii}	2.52 (4)
Ti3—O3	1.9332 (7)	Ga5—O7	1.89 (2)
Ti3—O4	1.8860 (11)	Ga5—O7^{i}	1.89 (2)

Symmetry codes: (i) $x, y, 1+z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, -\frac{1}{2}-z$; (iv) $x, y, z-1$; (v) $y, -x, -z$; (vi) $y, 1-x, -z$; (vii) $y, 1-x, 1-z$; (viii) $-y, x, z$.

Table *S*7. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for sample–III*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	x	y	z	$U_{\rm eq}$
K1	0.314 (5)	0	0	0.226 (3)	0.085 (5)
Ga1	0.7059 (19)	0.11781 (2)	0.16271 (2)	0.5	0.00546 (8)
Al1	0.286 (2)	0.11781	0.16271	0.5	0.00546
Ga2	0.475 (9)	0.20407 (2)	0.31096 (2)	0	0.00668 (10)
Al2	0.35 (2)	0.20407	0.31096	0	0.00668
Ti2	0.17 (2)	0.20407	0.31096	0	0.00668
Ti3	0.69 (2)	0.22114 (3)	0.03631 (3)	0	0.00678 (10)
Ga3	0.105 (10)	0.22114	0.03631	0	0.00678
Al3	0.20 (2)	0.22114	0.03631	0	0.00678
Ti4	0.997 (3)	0.12029 (3)	0.54304 (3)	0	0.01008 (10)
Ga4	0.003 (3)	0.12029	0.54304	0	0.01008
Ga5	0.0080 (11)	0.064 (2)	0.102 (2)	0.5	0.01
O1	1	0.40921 (10)	0.02046 (10)	0	0.0066 (4)
O2	1	0.39374 (10)	0.15235 (10)	0.5	0.0067 (4)
O3	1	0.28003 (10)	0.00222 (10)	0.5	0.0071 (4)
O4	1	0.26498 (10)	0.13137 (10)	0	0.0076 (4)
O5	1	0.18961 (10)	0.23608 (10)	0.5	0.0067 (4)
O6	1	0.15496 (10)	0.06837 (11)	0.5	0.0077 (4)
O7	1	0.06206 (10)	0.16859 (11)	0	0.0089 (4)

Table *S*8. *Anisotropic displacement parameters* (Å^2) *for sample–III*

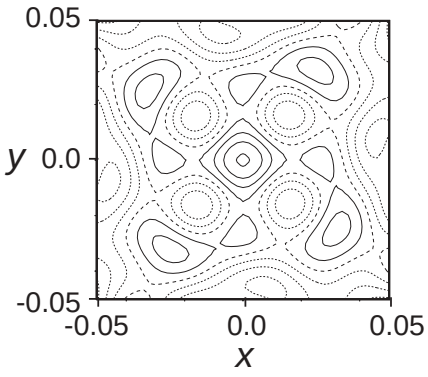
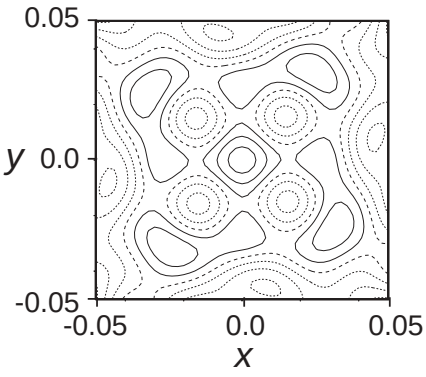
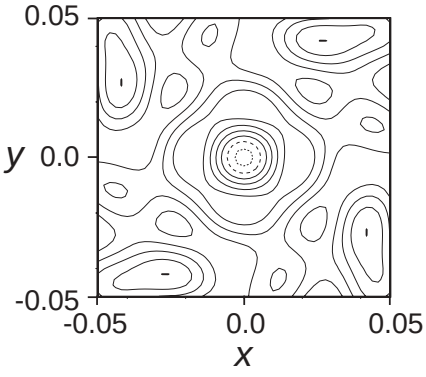
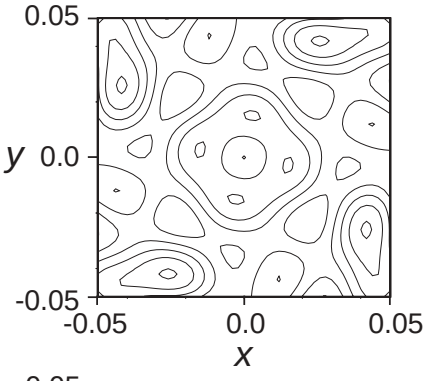
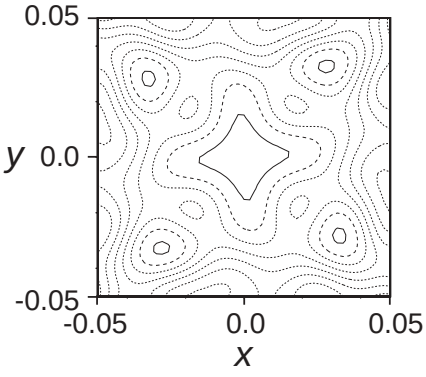
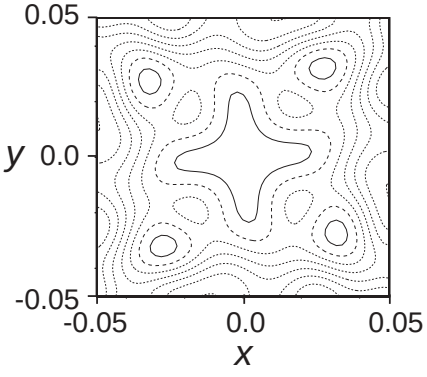
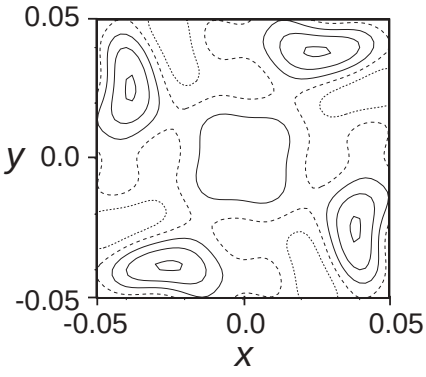
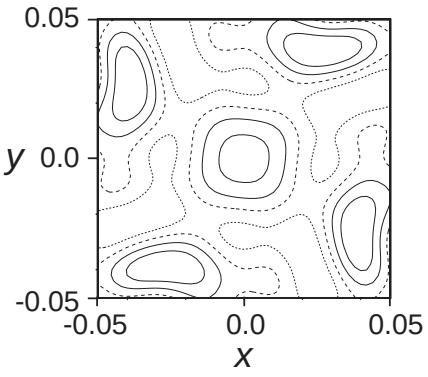
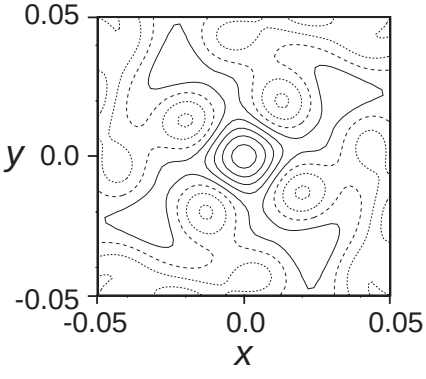
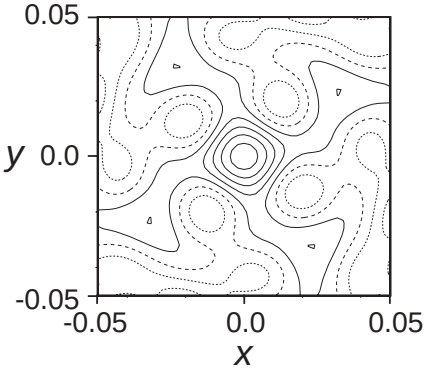
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.058 (4)	0.058 (4)	0.140 (12)	0	0	0
Ga1	0.00552 (13)	0.00609 (13)	0.00476 (13)	−0.00040 (10)	0	0
Ga2	0.00605 (16)	0.00833 (17)	0.00566 (18)	0.00032 (12)	0	0
Ti3	0.00868 (19)	0.00566 (17)	0.00600 (19)	−0.00025 (13)	0	0
Ti4	0.01162 (19)	0.01070 (18)	0.00792 (17)	−0.00049 (14)	0	0
O1	0.0075 (6)	0.0055 (6)	0.0069 (7)	−0.0010 (5)	0	0
O2	0.0059 (6)	0.0071 (6)	0.0070 (7)	0.0008 (5)	0	0
O3	0.0061 (6)	0.0078 (6)	0.0075 (7)	0.0028 (5)	0	0
O4	0.0091 (7)	0.0052 (6)	0.0086 (7)	−0.0011 (5)	0	0
O5	0.0059 (6)	0.0058 (6)	0.0085 (7)	−0.0004 (5)	0	0
O6	0.0054 (6)	0.0094 (7)	0.0084 (7)	0.0011 (5)	0	0
O7	0.0073 (6)	0.0121 (7)	0.0073 (7)	0.0023 (6)	0	0

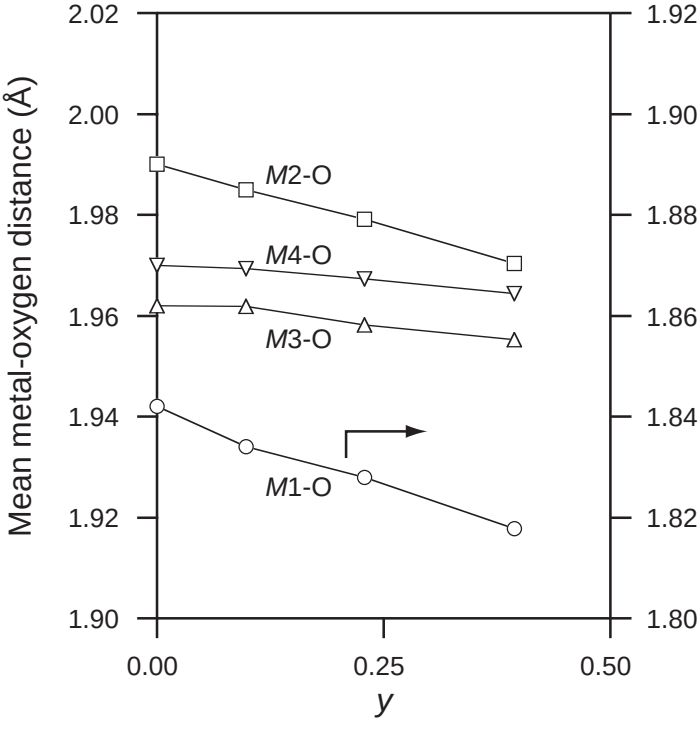
Table *S*9. *Geometric parameters (Å, °) for sample–III*

Ga1—O5	1.8487 (18)	Ti3—O6^{iv}	1.9919 (12)
Ga1—O6	1.8260 (19)	Ti3—O6	1.9919 (12)
Ga1—O7	1.7981 (11)	Ti3—O7^{v}	2.009 (2)
Ga1—O7^{i}	1.7981 (11)	Ti4—O1^{iii}	1.9504 (12)
Ga2—O2^{ii}	1.8813 (18)	Ti4—O1^{ii}	1.9504 (12)
Ga2—O4^{iii}	1.8983 (11)	Ti4—O1^{vi}	1.9928 (19)
Ga2—O4^{ii}	1.8983 (11)	Ti4—O2^{vi}	1.9605 (12)
Ga2—O5^{iv}	2.0249 (12)	Ti4—O2^{vii}	1.9605 (12)
Ga2—O5	2.0249 (12)	Ti4—O3^{ii}	1.9716 (19)
Ga2—O5^{ii}	2.0937 (18)	Ga5—O6	1.75 (4)
Ti3—O3^{iv}	1.9276 (12)	Ga5—O6^{viii}	2.57 (4)
Ti3—O3	1.9276 (12)	Ga5—O7	1.91 (3)
Ti3—O4	1.8850 (18)	Ga5—O7^{i}	1.91 (3)

Symmetry codes: (i) $x, y, 1+z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (iii) $\frac{1}{2}-x, \frac{1}{2}-y, -\frac{1}{2}-z$; (iv) $x, y, z-1$; (v) $y, -x, -z$; (vi) $y, 1-x, -z$; (vii) $y, 1-x, 1-z$; (viii) $-y, x, z$.

Supplementary data: Difference Fourier maps

	harmonic model	anharmonic model
sample I z=0.5 contour intervals: 0.2 e/Å		
sample II z=0 contour intervals: 0.2 e/Å		
z=0.5 contour intervals: 0.2 e/Å		
sample III z=0 contour intervals: 0.4 e/Å		
z=0.5 contour intervals: 0.4 e/Å		



Composition dependence of the mean metal-oxygen distance in coordination polyhedra. y is the parameter for the chemical composition of the crystal $K_x(Ga_{1-y}Al_y)_{2+x}Ti_{2-x}O_7$ ($x \approx 0.14$).