Supplementary data

Table 1. *Polarization vectors of the five different irrep distortions present in the Pnma structure of $SrZrO_3$ at 20K (Howard* et al.*, 2000). The table shows an asymmetric unit of the Pnam structure with the positions corresponding to the parent structure. Then, the atomic displacements (in relative units) for the polarization vectors (normalized to 1 Å) of the different irrep distortions are listed for the same asymmetric unit, together with their amplitudes. Atomic displacements are expressed in relative units with respect to the corresponding supercell of the reported parent phase (a=5.8710, b=8.3028,c=5.871)*

Reference Structure

Zr	1	4a	0.000000	0.000000	0.000000
Sr	2	4c	0.500000	0.250000	0.000000
O	3	8d	0.250000	0.000000	0.750000
O	3_2	4c	0.500000	0.750000	0.500000

Mode R4+

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	0.0000	-0.0301	0.0000
O3_2	0.0000	0.0000	-0.0602

Mode R5+

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0851
O3	0.0000	0.0009	0.0000
O3_2	0.0000	0.0000	-0.0019

Mode X5+

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0725	0.0000	0.0000
O3	0.0000	0.0000	0.0000
O3_2	0.0447	0.0000	0.0000

Mode M2+

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	-0.0426	0.0000	0.0426
O3_2	0.0000	0.0000	0.0000

Mode M3+

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	-0.0426	0.0000	-0.0426
O3_2	0.0000	0.0000	0.0000

Amm2 structure of BaTiO3 at 190K (Kwei et al. (1993). J. Phys. Chem. 97(10), 2368-2377)

Symmetry mode analysis

High symmetry structure

```
221
4.006 4.006 4.006 90 90 90
3
Ba       1        1a       0.000000         0.000000         0.000000
Ti       1        1b       0.500000         0.500000         0.500000
O        1        3c       0.500000         0.000000         0.500000
```

Low symmetry structure

```
38
3.9828 5.6745 5.6916 90 90 90
4
Ba       1        2a       0.000000         0.000000         0.000000
Ti       1        2b       0.500000         0.000000         0.517000
O        1        2a       0.000000         0.000000         0.489000
O        2        4e       0.500000         0.256100         0.234300
```

Transformation matrix

```
[      0      1      1  ] [       0]
[      0     -1      1  ] [       0]
[      1      0      0  ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
038
4.006000 5.665339 5.665339 90.000000 90.000000 90.000000
4
Ba       1        2a       0.000000         0.000000         0.000000
Ti       1        2b       0.500000         0.000000         0.500000
O        1        4e       0.500000         0.250000         0.250000
O        1_2      2a       0.000000         0.000000         0.500000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
2a	(0,0,z)	Ba1	(0.000000,0.000000,0.000000)	Ba1	(0.000000,0.000000,0.000000)
2b	(1/2,0,z)	Ti1	(0.500000,0.000000,0.500000)	Ti1	(0.500000,0.000000,0.517000)

4e	(1/2,y,z)	O1	(0.500000,0.250000,0.250000)	O2	(0.500000,0.256100,0.234300)
2a	(0,0,z)	O1_2	(0.000000,0.000000,0.500000)	O1	(0.000000,0.000000,0.489000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ba1	0.0000	0.0000	0.0000	0.0000
2b	(1/2,0,z)	Ti1	0.0000	0.0000	0.0170	0.0963
4e	(1/2,y,z)	O1	0.0000	0.0061	-0.0157	0.0954
2a	(0,0,z)	O1_2	0.0000	0.0000	-0.0110	0.0623

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.0963 Å
Total distortion amplitude: 0.1771 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.00508)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Ba1	(0.000000,0.000000,0.000000)	Ba1	(0.000000,0.000000,0.005080)
2b	(1/2,0,z)	Ti1	(0.500000,0.000000,0.500000)	Ti1	(0.500000,0.000000,0.522080)
4e	(1/2,y,z)	O1	(0.500000,0.250000,0.250000)	O2	(0.500000,0.256100,0.239380)
2a	(0,0,z)	O1_2	(0.000000,0.000000,0.500000)	O1	(0.000000,0.000000,0.494080)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ba1	0.0000	0.0000	0.0051	0.0288
2b	(1/2,0,z)	Ti1	0.0000	0.0000	0.0221	0.1251
4e	(1/2,y,z)	O1	0.0000	0.0061	-0.0106	0.0694
2a	(0,0,z)	O1_2	0.0000	0.0000	-0.0059	0.0335

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1251 Å
Total distortion amplitude: 0.1650 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	3*c*	**GM4-(2) GM5-(1)**
Ti1	1*b*	**GM4-(1)**
Ba1	1*a*	**GM4-(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM4-	(a,a,0)	Amm2 (38)	4	0.1649
(0,0,0)	GM5-	(0,a,-a)	Amm2 (38)	1	0.0056

Global distortion: 0.1650 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM4-

GM4- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.176512

GM4- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.176512

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

GM4- Mode O1 2

Atom	δx	δy	δz

O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

Irrep GM5-

GM5- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.062406	-0.062406
O1_2	0.000000	0.000000	0.124813

K-vector: GM = (0,0,0)

Irrep: GM4-

Direction: (a,a,0)

Isotropy Subgroup: 38 Amm2 C2v-14

Transformation matrix:

```
[      0      1      1 ] [      0]
[      0     -1      1 ] [      0]
[      1      0      0 ] [      0]
```

The amplitude of this distortion is:
A_{GM4-} = 0.1649 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ba1 1	Ti1 1	O1 1	O1 2
0.1745	0.7585	-0.2536	-0.5744

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ba1	0.0000	0.0000	0.0308
Ti1	0.0000	0.0000	0.1339
O1	0.0000	0.0349	-0.0665

O1_2	0.0000	0.0000	-0.0317

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM5-

Direction: (0,a,-a)

Isotropy Subgroup: 38 Amm2 C2v-14

Transformation matrix:

```
[      0       1       1 ] [       0]
[      0      -1       1 ] [       0]
[      1       0       0 ] [       0]
```

The amplitude of this distortion is:
A_{GM5-} = 0.0056 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O1 1
-0.0056

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ba1	0.0000	0.0000	0.0000
Ti1	0.0000	0.0000	0.0000
O1	0.0000	0.0624	0.0624
O1_2	0.0000	0.0000	-0.1248

Virtual structure with only this symmetry component of the distortion frozen.

Gd2(MO4)2 - Pba2 - RT (Jeitschko, Acta Cryst. (1972). B28, 60-76)

Symmetry mode analysis

High symmetry structure

```
113
7.3930 7.3930 10.6700 90.00 90.00 90.00
7
Gd       1       4e      0.687440        0.812560        0.737620
Mo       1       4e      0.706630        0.793370        0.356950
Mo       2       2a      0.500000        0.500000        0.000000
O        1       4e      0.695200        0.804800        0.519500
O        2       4e      0.128900        0.371100        0.310900
O        3       8f      0.276100        0.498300        0.700500
O        4       8f      0.314700        0.539300        0.095500
```

Low symmetry structure

```
32
10.3881 10.4194 10.7007 90 90 90
17
Gd       1       4c      0.187760        0.495360        0.737720
Gd       2       4c      0.492980        0.312340        0.263150
Mo       1       4c      0.205690        0.488980        0.357260
Mo       2       4c      0.002890        0.206490        0.642570
Mo       3       4c      0.242300        0.242850        0.000000
O        1       4c      0.192100        0.488200        0.518600
O        2       4c      0.480100        0.305300        0.482500
O        3       4c      0.128700        0.006900        0.311200
O        4       4c      0.494000        0.128000        0.689900
O        5       4c      0.157900        0.155700        0.681500
O        6       4c      0.157100        0.336000        0.307400
O        7       4c      0.384000        0.383700        0.719100
O        8       4c      0.384800        0.114500        0.294100
O        9       4c      0.125500        0.170800        0.093700
O        10      4c      0.317400        0.126400        0.907400
O        11      4c      0.354500        0.319700        0.098400
O        12      4c      0.170400        0.357100        0.902400
```

Transformation matrix

```
[     1     1     0 ] [       0]
[    -1     1     0 ] [     1/2]
[     0     0     1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
032
10.455281 10.455281 10.670000 90.000000 90.000000 90.000000
17
Gd       1       4c      0.187440        0.500000        0.737620
Gd       1_2     4c      0.000000        0.812560        0.262380
Mo       1       4c      0.206630        0.500000        0.356950
Mo       1_2     4c      0.000000        0.793370        0.643050
Mo       2       4c      0.250000        0.250000        0.000000
O        1       4c      0.195200        0.500000        0.519500
O        1_2     4c      0.000000        0.804800        0.480500
O        2       4c      0.128900        0.000000        0.310900
O        2_2     4c      0.500000        0.871100        0.689100
O        3       4c      0.138900        0.137200        0.700500
O        3_2     4c      0.361100        0.362800        0.700500
O        3_3     4c      0.637200        0.861100        0.299500
O        3_4     4c      0.862800        0.638900        0.299500
O        4       4c      0.137700        0.177000        0.095500
O        4_2     4c      0.362300        0.323000        0.095500
O        4_3     4c      0.677000        0.862300        0.904500
O        4_4     4c      0.823000        0.637700        0.904500
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4c	(x,y,z)	Gd1	(0.187440,0.500000,0.737620)	Gd1	(0.187760,0.495360,0.737720)
4c	(x,y,z)	Gd1_2	(0.000000,0.812560,0.262380)	Gd2	(0.007020,0.812340,0.263150)
4c	(x,y,z)	Mo1	(0.206630,0.500000,0.356950)	Mo1	(0.205690,0.488980,0.357260)
4c	(x,y,z)	Mo1_2	(0.000000,0.793370,0.643050)	Mo2	(0.997110,0.793510,0.642570)
4c	(x,y,z)	Mo2	(0.250000,0.250000,0.000000)	Mo3	(0.242300,0.242850,0.000000)
4c	(x,y,z)	O1	(0.195200,0.500000,0.519500)	O1	(0.192100,0.488200,0.518600)
4c	(x,y,z)	O1_2	(0.000000,0.804800,0.480500)	O2	(0.019900,0.805300,0.482500)
4c	(x,y,z)	O2	(0.128900,0.000000,0.310900)	O3	(0.128700,0.006900,0.311200)
4c	(x,y,z)	O2_2	(0.500000,0.871100,0.689100)	O4	(0.506000,0.872000,0.689900)
4c	(x,y,z)	O3	(0.138900,0.137200,0.700500)	O5	(0.157900,0.155700,0.681500)

4c	(x,y,z)	O3_2	(0.361100,0.362800,0.700500)	O7	(0.384000,0.383700,0.719100)
4c	(x,y,z)	O3_3	(0.637200,0.861100,0.299500)	O8	(0.615200,0.885500,0.294100)
4c	(x,y,z)	O3_4	(0.862800,0.638900,0.299500)	O6	(0.842900,0.664000,0.307400)
4c	(x,y,z)	O4	(0.137700,0.177000,0.095500)	O9	(0.125500,0.170800,0.093700)
4c	(x,y,z)	O4_2	(0.362300,0.323000,0.095500)	O11	(0.354500,0.319700,0.098400)
4c	(x,y,z)	O4_3	(0.677000,0.862300,0.904500)	O10	(0.682600,0.873600,0.907400)
4c	(x,y,z)	O4_4	(0.823000,0.637700,0.904500)	O12	(0.829600,0.642900,0.902400)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4c	(x,y,z)	Gd1	0.0003	-0.0046	0.0001	0.0486
4c	(x,y,z)	Gd1_2	0.0070	-0.0002	0.0008	0.0739
4c	(x,y,z)	Mo1	-0.0009	-0.0110	0.0003	0.1157
4c	(x,y,z)	Mo1_2	-0.0029	0.0001	-0.0005	0.0307
4c	(x,y,z)	Mo2	-0.0077	-0.0072	0.0000	0.1099
4c	(x,y,z)	O1	-0.0031	-0.0118	-0.0009	0.1279
4c	(x,y,z)	O1_2	0.0199	0.0005	0.0020	0.2092
4c	(x,y,z)	O2	-0.0002	0.0069	0.0003	0.0722
4c	(x,y,z)	O2_2	0.0060	0.0009	0.0008	0.0640
4c	(x,y,z)	O3	0.0190	0.0185	-0.0190	0.3435
4c	(x,y,z)	O3_2	0.0229	0.0209	0.0186	0.3801
4c	(x,y,z)	O3_3	-0.0220	0.0244	-0.0054	0.3483
4c	(x,y,z)	O3_4	-0.0199	0.0251	0.0079	0.3453
4c	(x,y,z)	O4	-0.0122	-0.0062	-0.0018	0.1444
4c	(x,y,z)	O4_2	-0.0078	-0.0033	0.0029	0.0938
4c	(x,y,z)	O4_3	0.0056	0.0113	0.0029	0.1354
4c	(x,y,z)	O4_4	0.0066	0.0052	-0.0021	0.0907

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.3801 Å
Total distortion amplitude: 1.6284 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.00041)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4c	(x,y,z)	Gd1	(0.187440,0.500000,0.737620)	Gd1	(0.187760,0.495360,0.737314)
4c	(x,y,z)	Gd1_2	(0.000000,0.812560,0.262380)	Gd2	(0.007020,0.812340,0.262744)
4c	(x,y,z)	Mo1	(0.206630,0.500000,0.356950)	Mo1	(0.205690,0.488980,0.356854)
4c	(x,y,z)	Mo1_2	(0.000000,0.793370,0.643050)	Mo2	(0.997110,0.793510,0.642164)
4c	(x,y,z)	Mo2	(0.250000,0.250000,0.000000)	Mo3	(0.242300,0.242850,0.999594)
4c	(x,y,z)	O1	(0.195200,0.500000,0.519500)	O1	(0.192100,0.488200,0.518194)
4c	(x,y,z)	O1_2	(0.000000,0.804800,0.480500)	O2	(0.019900,0.805300,0.482094)
4c	(x,y,z)	O2	(0.128900,0.000000,0.310900)	O3	(0.128700,0.006900,0.310794)
4c	(x,y,z)	O2_2	(0.500000,0.871100,0.689100)	O4	(0.506000,0.872000,0.689494)
4c	(x,y,z)	O3	(0.138900,0.137200,0.700500)	O5	(0.157900,0.155700,0.681094)
4c	(x,y,z)	O3_2	(0.361100,0.362800,0.700500)	O7	(0.384000,0.383700,0.718694)
4c	(x,y,z)	O3_3	(0.637200,0.861100,0.299500)	O8	(0.615200,0.885500,0.293694)
4c	(x,y,z)	O3_4	(0.862800,0.638900,0.299500)	O6	(0.842900,0.664000,0.306994)
4c	(x,y,z)	O4	(0.137700,0.177000,0.095500)	O9	(0.125500,0.170800,0.093294)
4c	(x,y,z)	O4_2	(0.362300,0.323000,0.095500)	O11	(0.354500,0.319700,0.097994)
4c	(x,y,z)	O4_3	(0.677000,0.862300,0.904500)	O10	(0.682600,0.873600,0.906994)
4c	(x,y,z)	O4_4	(0.823000,0.637700,0.904500)	O12	(0.829600,0.642900,0.901994)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4c	(x,y,z)	Gd1	0.0003	-0.0046	-0.0003	0.0487
4c	(x,y,z)	Gd1_2	0.0070	-0.0002	0.0004	0.0735
4c	(x,y,z)	Mo1	-0.0009	-0.0110	-0.0001	0.1156
4c	(x,y,z)	Mo1_2	-0.0029	0.0001	-0.0009	0.0317
4c	(x,y,z)	Mo2	-0.0077	-0.0072	-0.0004	0.1099
4c	(x,y,z)	O1	-0.0031	-0.0118	-0.0013	0.1283
4c	(x,y,z)	O1_2	0.0199	0.0005	0.0016	0.2088
4c	(x,y,z)	O2	-0.0002	0.0069	-0.0001	0.0722
4c	(x,y,z)	O2_2	0.0060	0.0009	0.0004	0.0636
4c	(x,y,z)	O3	0.0190	0.0185	-0.0194	0.3460
4c	(x,y,z)	O3_2	0.0229	0.0209	0.0182	0.3778
4c	(x,y,z)	O3_3	-0.0220	0.0244	-0.0058	0.3490
4c	(x,y,z)	O3_4	-0.0199	0.0251	0.0075	0.3443
4c	(x,y,z)	O4	-0.0122	-0.0062	-0.0022	0.1450
4c	(x,y,z)	O4_2	-0.0078	-0.0033	0.0025	0.0925
4c	(x,y,z)	O4_3	0.0056	0.0113	0.0025	0.1345
4c	(x,y,z)	O4_4	0.0066	0.0052	-0.0025	0.0918

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.3778 Å
Total distortion amplitude: 1.6278 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3 O4	8*f*	GM1(3) GM3(3) **M2M4(6)**
Mo1 O2 Gd1 O1	4*e*	GM1(2) GM3(2) **M2M4(2)**
Mo2	2*a*	GM3(1) **M2M4(2)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1	(a)	P-42_1m (113)	14	0.1538
(0,0,0)	GM3	(a)	Cmm2 (35)	15	0.0716
(1/2,1/2,0)	M2M4	(a,b)	Pba2 (32)	22	1.6191

Global distortion: 1.6280 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1

GM1 Mode Gd1 1

Atom	δx	δy	δz
Gd1	0.000000	0.000000	-0.033135
Gd1_2	0.000000	0.000000	0.033135

GM1 Mode Gd1 2

Atom	δx	δy	δz
Gd1	-0.033816	0.000000	0.000000
Gd1_2	0.000000	0.033816	-0.000000

GM1 Mode Mo1 1

Atom	δx	δy	δz
Mo1	0.000000	0.000000	-0.033135
Mo1_2	0.000000	0.000000	0.033135

GM1 Mode Mo1 2

Atom	δx	δy	δz
Mo1	-0.033816	0.000000	0.000000
Mo1_2	0.000000	0.033816	-0.000000

GM1 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	-0.033135
O1_2	0.000000	0.000000	0.033135

GM1 Mode O1 2

Atom	δx	δy	δz
O1	-0.033816	0.000000	0.000000
O1_2	0.000000	0.033816	-0.000000

GM1 Mode O2 1

Atom	δx	δy	δz
O2	0.000000	0.000000	-0.033135
O2_2	0.000000	0.000000	0.033135

GM1 Mode O2 2

Atom	δx	δy	δz
O2	-0.033816	0.000000	0.000000
O2_2	0.000000	0.033816	-0.000000

GM1 Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.023430
O3_2	0.000000	0.000000	0.023430
O3_3	0.000000	0.000000	-0.023430
O3_4	0.000000	0.000000	-0.023430

GM1 Mode O3 2

Atom	δx	δy	δz
O3	0.016908	0.016908	-0.000000
O3_2	-0.016908	-0.016908	0.000000
O3_3	0.016908	-0.016908	0.000000
O3_4	-0.016908	0.016908	-0.000000

GM1 Mode O3 3

Atom	δx	δy	δz
O3	-0.016908	0.016908	-0.000000
O3_2	0.016908	-0.016908	0.000000
O3_3	0.016908	0.016908	-0.000000
O3_4	-0.016908	-0.016908	0.000000

GM1 Mode O4 1

Atom	δx	δy	δz
O4	0.000000	0.000000	0.023430
O4_2	0.000000	0.000000	0.023430
O4_3	0.000000	0.000000	-0.023430
O4_4	0.000000	0.000000	-0.023430

GM1 Mode O4 2

Atom	δx	δy	δz
O4	0.016908	0.016908	-0.000000
O4_2	-0.016908	-0.016908	0.000000
O4_3	0.016908	-0.016908	0.000000
O4_4	-0.016908	0.016908	-0.000000

GM1 Mode O4 3

Atom	δx	δy	δz
O4	-0.016908	0.016908	-0.000000
O4_2	0.016908	-0.016908	0.000000
O4_3	0.016908	0.016908	-0.000000
O4_4	-0.016908	-0.016908	0.000000

Irrep GM3

GM3 Mode Gd1 1

Atom	δx	δy	δz
Gd1	0.033816	-0.000000	-0.000000
Gd1_2	0.000000	0.033816	-0.000000

GM3 Mode Gd1 2

Atom	δx	δy	δz
Gd1	0.000000	0.000000	0.033135
Gd1_2	0.000000	0.000000	0.033135

GM3 Mode Mo1 1

Atom	δx	δy	δz
Mo1	0.033816	-0.000000	-0.000000
Mo1_2	0.000000	0.033816	-0.000000

GM3 Mode Mo1 2

Atom	δx	δy	δz
Mo1	0.000000	0.000000	0.033135
Mo1_2	0.000000	0.000000	0.033135

GM3 Mode Mo2 1

Atom	δx	δy	δz
Mo2	0.000000	0.000000	0.046860

GM3 Mode O1 1

Atom	δx	δy	δz
O1	0.033816	-0.000000	-0.000000
O1_2	0.000000	0.033816	-0.000000

GM3 Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.033135
O1_2	0.000000	0.000000	0.033135

GM3 Mode O2 1

Atom	δx	δy	δz
O2	0.033816	-0.000000	-0.000000
O2_2	0.000000	0.033816	-0.000000

GM3 Mode O2 2

Atom	δx	δy	δz
O2	0.000000	0.000000	0.033135
O2_2	0.000000	0.000000	0.033135

GM3 Mode O3 1

Atom	δx	δy	δz
O3	-0.016908	0.016908	-0.000000
O3_2	0.016908	-0.016908	0.000000
O3_3	-0.016908	-0.016908	0.000000
O3_4	0.016908	0.016908	-0.000000

GM3 Mode O3 2

Atom	δx	δy	δz
O3	0.016908	0.016908	-0.000000
O3_2	-0.016908	-0.016908	0.000000
O3_3	-0.016908	0.016908	-0.000000
O3_4	0.016908	-0.016908	0.000000

GM3 Mode O3 3

Atom	δx	δy	δz
O3	0.000000	0.000000	0.023430
O3_2	0.000000	0.000000	0.023430
O3_3	0.000000	0.000000	0.023430
O3_4	0.000000	0.000000	0.023430

GM3 Mode O4 1

Atom	δx	δy	δz
O4	-0.016908	0.016908	-0.000000
O4_2	0.016908	-0.016908	0.000000
O4_3	-0.016908	-0.016908	0.000000
O4_4	0.016908	0.016908	-0.000000

GM3 Mode O4 2

Atom	δx	δy	δz
O4	0.016908	0.016908	-0.000000
O4_2	-0.016908	-0.016908	0.000000
O4_3	-0.016908	0.016908	-0.000000
O4_4	0.016908	-0.016908	0.000000

GM3 Mode O4 3

Atom	δx	δy	δz
O4	0.000000	0.000000	0.023430
O4_2	0.000000	0.000000	0.023430
O4_3	0.000000	0.000000	0.023430
O4_4	0.000000	0.000000	0.023430

Irrep M2M4

M2M4 Mode Gd1 1

Atom	δx	δy	δz
Gd1	0.000000	-0.047823	0.000000
Gd1_2	0.000000	0.000000	0.000000

M2M4 Mode Gd1 2

Atom	δx	δy	δz
Gd1	0.000000	0.000000	0.000000
Gd1_2	0.047823	-0.000000	-0.000000

M2M4 Mode Mo1 1

Atom	δx	δy	δz
Mo1	0.000000	-0.047823	0.000000
Mo1_2	0.000000	0.000000	0.000000

M2M4 Mode Mo1 2

Atom	δx	δy	δz
Mo1	0.000000	0.000000	0.000000
Mo1_2	0.047823	-0.000000	-0.000000

M2M4 Mode Mo2 1

Atom	δx	δy	δz
Mo2	-0.033816	0.033816	-0.000000

M2M4 Mode Mo2 2

Atom	δx	δy	δz
Mo2	-0.033816	-0.033816	0.000000

M2M4 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.047823	0.000000
O1_2	0.000000	0.000000	0.000000

M2M4 Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.047823	-0.000000	-0.000000

M2M4 Mode O2 1

Atom	δx	δy	δz
O2	0.000000	0.000000	0.000000
O2_2	-0.047823	0.000000	0.000000

M2M4 Mode O2 2

Atom	δx	δy	δz
O2	0.000000	0.047823	-0.000000
O2_2	0.000000	0.000000	0.000000

M2M4 Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	0.000000	0.000000
O3_3	0.023911	0.023911	-0.000000
O3_4	0.023911	0.023911	-0.000000

M2M4 Mode O3 2

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	0.000000	0.000000
O3_3	0.023911	-0.023911	0.000000
O3_4	0.023911	-0.023911	0.000000

M2M4 Mode O3 3

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	0.000000	0.000000
O3_3	0.000000	0.000000	-0.033135
O3_4	0.000000	0.000000	0.033135

M2M4 Mode O3 4

Atom	δx	δy	δz
O3	-0.023911	0.023911	-0.000000
O3_2	-0.023911	0.023911	-0.000000
O3_3	0.000000	0.000000	0.000000
O3_4	0.000000	0.000000	0.000000

M2M4 Mode O3 5

Atom	δx	δy	δz
O3	0.000000	0.000000	0.033135
O3_2	0.000000	0.000000	-0.033135
O3_3	0.000000	0.000000	0.000000
O3_4	0.000000	0.000000	0.000000

M2M4 Mode O3 6

Atom	δx	δy	δz
O3	0.023911	0.023911	-0.000000
O3_2	0.023911	0.023911	-0.000000
O3_3	0.000000	0.000000	0.000000
O3_4	0.000000	0.000000	0.000000

M2M4 Mode O4 1

Atom	δx	δy	δz
O4	0.000000	0.000000	0.000000
O4_2	0.000000	0.000000	0.000000
O4_3	0.023911	0.023911	-0.000000
O4_4	0.023911	0.023911	-0.000000

M2M4 Mode O4 2

Atom	δx	δy	δz
O4	0.000000	0.000000	0.000000
O4_2	0.000000	0.000000	0.000000
O4_3	0.023911	-0.023911	0.000000
O4_4	0.023911	-0.023911	0.000000

M2M4 Mode O4 3

Atom	δx	δy	δz
O4	0.000000	0.000000	0.000000
O4_2	0.000000	0.000000	0.000000
O4_3	0.000000	0.000000	-0.033135
O4_4	0.000000	0.000000	0.033135

M2M4 Mode O4 4

Atom	δx	δy	δz
O4	-0.023911	0.023911	-0.000000
O4_2	-0.023911	0.023911	-0.000000
O4_3	0.000000	0.000000	0.000000
O4_4	0.000000	0.000000	0.000000

M2M4 Mode O4 5

Atom	δx	δy	δz
O4	0.000000	0.000000	0.033135
O4_2	0.000000	0.000000	-0.033135
O4_3	0.000000	0.000000	0.000000
O4_4	0.000000	0.000000	0.000000

M2M4 Mode O4 6

Atom	δx	δy	δz
O4	0.023911	0.023911	-0.000000
O4_2	0.023911	0.023911	-0.000000
O4_3	0.000000	0.000000	0.000000
O4_4	0.000000	0.000000	0.000000

K-vector: GM = (0,0,0)

Irrep: GM1

Direction: (a)

Isotropy Subgroup: 113 P-42_1m D2d-3

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:

A_{GM1}= 0.1538 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Gd1 1	Gd1 2	Mo1 1	Mo1 2	O1 1	O1 2	O2 1	O2 2	O3 1	O3 2	O3 3	O4 1	O4 2	O4 3
0.0657	-0.0519	-0.0775	0.1038	0.2846	0.3461	0.0491	0.1058	-0.2012	-0.3702	-0.0625	0.0208	-0.6923	0.3173

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Gd1	0.0018	-0.0000	-0.0022
Gd1_2	0.0000	-0.0018	0.0022
Mo1	-0.0035	0.0000	0.0026
Mo1_2	0.0000	0.0035	-0.0026
Mo2	0.0000	0.0000	0.0000
O1	-0.0117	0.0000	-0.0094
O1_2	0.0000	0.0117	0.0094
O2	-0.0036	0.0000	-0.0016
O2_2	0.0000	0.0036	0.0016
O3	-0.0052	-0.0073	-0.0047
O3_2	0.0052	0.0073	-0.0047
O3_3	-0.0073	0.0052	0.0047
O3_4	0.0073	-0.0052	0.0047
O4	-0.0171	-0.0063	0.0005
O4_2	0.0171	0.0063	0.0005
O4_3	-0.0063	0.0171	-0.0005
O4_4	0.0063	-0.0171	-0.0005

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM3

Direction: (a)

Isotropy Subgroup: 35 Cmm2 C2v-11

Transformation matrix:

```
[     1     -1      0 ] [       0]
[     1      1      0 ] [     1/2]
[     0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{GM3}= 0.0716 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Gd1 1	Gd1 2	Mo1 1	Mo1 2	Mo2 1	O1 1	O1 2	O2 1	O2 2	O3 1	O3 2	O3 3	O4 1	O4 2	O4 3
0.0207	0.0122	-0.1652	-0.2069	-0.1210	-0.5368	0.0607	0.1445	0.0607	0.4439	-0.5059	0.0709	-0.3717	-0.0206	0.0411

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Gd1	0.0007	-0.0000	0.0004
Gd1_2	0.0000	0.0007	0.0004
Mo1	-0.0056	0.0000	-0.0069
Mo1_2	0.0000	-0.0056	-0.0069
Mo2	0.0000	0.0000	-0.0057
O1	-0.0182	0.0000	0.0020
O1_2	0.0000	-0.0182	0.0020
O2	0.0049	-0.0000	0.0020
O2_2	0.0000	0.0049	0.0020
O3	-0.0161	-0.0010	0.0017

O3_2	0.0161	0.0010	0.0017
O3_3	0.0010	-0.0161	0.0017
O3_4	-0.0010	0.0161	0.0017
O4	0.0059	-0.0066	0.0010
O4_2	-0.0059	0.0066	0.0010
O4_3	0.0066	0.0059	0.0010
O4_4	-0.0066	-0.0059	0.0010

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: M = (1/2,1/2,0)

Irrep: M2M4

Direction: (a,b)

Isotropy Subgroup: 32 Pba2 C2v-8

Transformation matrix:

```
[     1     1     0 ] [      0]
[    -1     1     0 ] [    1/2]
[     0     0     1 ] [      0]
```

The amplitude of this distortion is:
A_{M2M4}= 1.6191 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Gd1 1	Gd1 2	Mo1 1	Mo1 2	Mo2 1	Mo2 2	O1 1	O1 2	O2 1	O2 2	O3 1	O3 2	O3 3	O3 4	O3 5	O3 6	O4 1	O4 2	O4 3	O4
0.0599	0.0907	0.1423	-0.0373	0.0050	0.1356	0.1524	0.2570	-0.0775	0.0891	0.0491	-0.5902	0.1240	-0.0161	-0.3504	0.5250	0.1853	-0.0278	-0.0466	0.0

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Gd1	0.0000	-0.0029	0.0000
Gd1_2	0.0043	-0.0000	-0.0000
Mo1	0.0000	-0.0068	0.0000
Mo1_2	-0.0018	0.0000	0.0000
Mo2	-0.0048	-0.0044	0.0000
O1	0.0000	-0.0073	0.0000
O1_2	0.0123	-0.0000	-0.0000
O2	0.0000	0.0043	-0.0000
O2_2	0.0037	-0.0000	-0.0000
O3	0.0129	0.0122	-0.0116
O3_2	0.0129	0.0122	0.0116
O3_3	-0.0129	0.0153	-0.0041
O3_4	-0.0129	0.0153	0.0041
O4	-0.0062	-0.0029	-0.0015
O4_2	-0.0062	-0.0029	0.0015
O4_3	0.0038	0.0051	0.0015
O4_4	0.0038	0.0051	-0.0015

Virtual structure with only this symmetry component of the distortion frozen.

KAlSi2O6-leucite-373K (Palmer et al. Amer. Miner. 82 (1997) 16)

Symmetry mode analysis

High symmetry structure

```
230
13.55038 13.55038 13.55038 90 90 90
3
K       1       16b     0.875000        0.375000        0.125000
T       1       48g     0.588100        0.375000        0.161900
O       1       96h     0.633000        0.280900        0.103800
```

Low symmetry structure

```
88
12.99517 12.99517 13.76451 90 90 90
10
K       1       16f     0.366300        0.365400        0.117100
T       1       16f     0.058200        0.396700        0.165400
T       2       16f     0.168500        0.612400        0.128000
T       3       16f     0.393300        0.640600        0.086300
O       1       16f     0.130800        0.313600        0.111100
O       2       16f     0.092700        0.510500        0.131000
O       3       16f     0.145500        0.679000        0.226900
O       4       16f     0.134200        0.683900        0.035800
O       5       16f     0.289200        0.577300        0.121200
O       6       16f     0.484100        0.617500        0.166500
```

Transformation matrix

```
[     1     0     0 ] [    1/2]
[     0     1     0 ] [      0]
[     0     0     1 ] [      0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
088
13.550380 13.550380 13.550380 90.000000 90.000000 90.000000
10
K       1       16f     0.375000        0.375000        0.125000
T       1       16f     0.088100        0.375000        0.161900
T       1_2     16f     0.911900        0.875000        0.338100
T       1_3     16f     0.661900        0.588100        0.375000
O       1       16f     0.133000        0.280900        0.103800
O       1_2     16f     0.867000        0.780900        0.396200
O       1_3     16f     0.603800        0.633000        0.280900
O       1_4     16f     0.103800        0.867000        0.719100
O       1_5     16f     0.780900        0.103800        0.633000
O       1_6     16f     0.219100        0.603800        0.867000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
16f	(x,y,z)	K1	(0.375000,0.375000,0.125000)	K1	(0.366300,0.365400,0.117100)
16f	(x,y,z)	T1	(0.088100,0.375000,0.161900)	T1	(0.058200,0.396700,0.165400)
16f	(x,y,z)	T1_2	(0.911900,0.875000,0.338100)	T3	(0.890600,0.856700,0.336300)
16f	(x,y,z)	T1_3	(0.661900,0.588100,0.375000)	T2	(0.668500,0.612400,0.372000)
16f	(x,y,z)	O1	(0.133000,0.280900,0.103800)	O1	(0.130800,0.313600,0.111100)
16f	(x,y,z)	O1_2	(0.867000,0.780900,0.396200)	O6	(0.867500,0.765900,0.416500)
16f	(x,y,z)	O1_3	(0.603800,0.633000,0.280900)	O3	(0.645500,0.679000,0.273100)
16f	(x,y,z)	O1_4	(0.103800,0.867000,0.719100)	O4	(0.066100,0.884200,0.714200)
16f	(x,y,z)	O1_5	(0.780900,0.103800,0.633000)	O5	(0.789200,0.077300,0.621200)

16f	(x,y,z)	O1_6	(0.219100,0.603800,0.867000)	O2	(0.260500,0.657300,0.881000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
16f	(x,y,z)	K1	-0.0087	-0.0096	-0.0079	0.2056
16f	(x,y,z)	T1	-0.0299	0.0217	0.0035	0.5029
16f	(x,y,z)	T1_2	-0.0213	-0.0183	-0.0018	0.3813
16f	(x,y,z)	T1_3	0.0066	0.0243	-0.0030	0.3436
16f	(x,y,z)	O1	-0.0022	0.0327	0.0073	0.4550
16f	(x,y,z)	O1_2	0.0005	-0.0150	0.0203	0.3421
16f	(x,y,z)	O1_3	0.0417	0.0460	-0.0078	0.8479
16f	(x,y,z)	O1_4	-0.0377	0.0172	-0.0049	0.5654
16f	(x,y,z)	O1_5	0.0083	-0.0265	-0.0118	0.4088
16f	(x,y,z)	O1_6	0.0414	0.0535	0.0140	0.9361

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.9361 Å
Total distortion amplitude: 4.8701 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	96*h*	GM1+(3) GM3+(6) **GM4+(9)**
T1	48*g*	GM1+(1) GM3+(3) **GM4+(5)**
K1	16*b*	GM3+(1) **GM4+(2)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Ia-3d (230)	4	0.4060
(0,0,0)	GM3+	(a,0)	I4_1/acd (142)	10	1.7219
(0,0,0)	GM4+	(0,0,a)	I4_1/a (88)	16	4.5374

Global distortion: 4.8701 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode T1 1

Atom	δx	δy	δz
T1	-0.010652	0.000000	0.010652
T1_2	0.010652	-0.000000	-0.010652
T1_3	0.010652	-0.010652	0.000000

GM1+ Mode O1 1

Atom	δx	δy	δz

O1	0.010652	-0.000000	-0.000000
O1_2	-0.010652	0.000000	0.000000
O1_3	0.000000	0.010652	-0.000000
O1_4	0.000000	-0.010652	0.000000
O1_5	0.000000	0.000000	0.010652
O1_6	0.000000	0.000000	-0.010652

GM1+ Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.010652	-0.000000
O1_2	0.000000	0.010652	-0.000000
O1_3	0.000000	0.000000	0.010652
O1_4	0.000000	0.000000	-0.010652
O1_5	0.010652	-0.000000	-0.000000
O1_6	-0.010652	0.000000	0.000000

GM1+ Mode O1 3

Atom	δx	δy	δz
O1	0.000000	0.000000	0.010652
O1_2	0.000000	0.000000	-0.010652
O1_3	0.010652	-0.000000	-0.000000
O1_4	0.010652	-0.000000	-0.000000
O1_5	0.000000	0.010652	-0.000000
O1_6	0.000000	0.010652	-0.000000

Irrep GM3+

GM3+ Mode K1 1

Atom	δx	δy	δz
K1	-0.018450	0.018450	-0.000000

GM3+ Mode T1 1

Atom	δx	δy	δz
T1	-0.007532	0.000000	0.007532
T1_2	0.007532	-0.000000	-0.007532
T1_3	-0.015064	0.015064	-0.000000

GM3+ Mode T1 2

Atom	δx	δy	δz
T1	-0.013046	0.000000	-0.013046
T1_2	0.013046	-0.000000	0.013046
T1_3	0.000000	0.000000	0.000000

GM3+ Mode T1 3

Atom	δx	δy	δz
T1	0.000000	0.018450	-0.000000
T1_2	0.000000	0.018450	-0.000000
T1_3	0.000000	0.000000	0.000000

GM3+ Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.015064
O1_2	0.000000	0.000000	-0.015064
O1_3	-0.007532	0.000000	0.000000
O1_4	-0.007532	0.000000	0.000000
O1_5	0.000000	-0.007532	0.000000
O1_6	0.000000	-0.007532	0.000000

GM3+ Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.013046	-0.000000
O1_4	0.000000	-0.013046	0.000000
O1_5	0.000000	0.000000	-0.013046
O1_6	0.000000	0.000000	0.013046

GM3+ Mode O1 3

Atom	δx	δy	δz
O1	0.000000	0.015064	-0.000000
O1_2	0.000000	0.015064	-0.000000
O1_3	0.000000	0.000000	-0.007532
O1_4	0.000000	0.000000	0.007532
O1_5	-0.007532	0.000000	0.000000
O1_6	0.007532	-0.000000	-0.000000

GM3+ Mode O1 4

Atom	δx	δy	δz
O1	0.000000	0.000000	-0.000000
O1_2	0.000000	0.000000	-0.000000
O1_3	0.000000	0.000000	0.013046
O1_4	0.000000	0.000000	-0.013046
O1_5	-0.013046	0.000000	0.000000
O1_6	0.013046	-0.000000	-0.000000

GM3+ Mode O1 5

Atom	δx	δy	δz
O1	0.015064	-0.000000	-0.000000
O1_2	-0.015064	0.000000	0.000000
O1_3	0.000000	-0.007532	0.000000
O1_4	0.000000	0.007532	-0.000000
O1_5	0.000000	0.000000	-0.007532
O1_6	0.000000	0.000000	0.007532

GM3+ Mode O1 6

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000

O1_2	0.000000	0.000000	-0.000000
O1_3	0.013046	-0.000000	-0.000000
O1_4	0.013046	-0.000000	-0.000000
O1_5	0.000000	-0.013046	0.000000
O1_6	0.000000	-0.013046	0.000000

Irrep GM4+

GM4+ Mode K1 1

Atom	δx	δy	δz
K1	-0.015064	-0.015064	0.015064

GM4+ Mode K1 2

Atom	δx	δy	δz
K1	0.010652	0.010652	0.021304

GM4+ Mode T1 1

Atom	δx	δy	δz
T1	0.013046	-0.000000	-0.013046
T1_2	0.013046	-0.000000	-0.013046
T1_3	0.000000	0.000000	0.000000

GM4+ Mode T1 2

Atom	δx	δy	δz
T1	0.000000	0.000000	0.000000
T1_2	0.000000	0.000000	0.000000
T1_3	0.018450	0.018450	-0.000000

GM4+ Mode T1 3

Atom	δx	δy	δz
T1	0.000000	0.000000	0.000000
T1_2	0.000000	0.000000	0.000000
T1_3	0.000000	0.000000	-0.026092

GM4+ Mode T1 4

Atom	δx	δy	δz
T1	0.000000	0.018450	-0.000000
T1_2	0.000000	-0.018450	0.000000
T1_3	0.000000	0.000000	0.000000

GM4+ Mode T1 5

Atom	δx	δy	δz
T1	-0.013046	0.000000	-0.013046
T1_2	-0.013046	0.000000	-0.013046
T1_3	0.000000	0.000000	0.000000

GM4+ Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000

O1_2	0.000000	0.000000	0.000000
O1_3	0.018450	-0.000000	-0.000000
O1_4	-0.018450	0.000000	0.000000
O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

GM4+ Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.000000	0.018450
O1_4	0.000000	0.000000	0.018450
O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

GM4+ Mode O1 3

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.018450	-0.000000
O1_6	0.000000	-0.018450	0.000000

GM4+ Mode O1 4

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.000000	0.018450
O1_6	0.000000	0.000000	0.018450

GM4+ Mode O1 5

Atom	δx	δy	δz
O1	0.000000	0.000000	0.018450
O1_2	0.000000	0.000000	0.018450
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

GM4+ Mode O1 6

Atom	δx	δy	δz
O1	0.018450	-0.000000	-0.000000
O1_2	0.018450	-0.000000	-0.000000
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000

O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

GM4+ Mode O1 7

Atom	δx	δy	δz
O1	0.000000	0.018450	-0.000000
O1_2	0.000000	-0.018450	0.000000
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

GM4+ Mode O1 8

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.018450	-0.000000	-0.000000
O1_6	0.018450	-0.000000	-0.000000

GM4+ Mode O1 9

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.000000
O1_3	0.000000	0.018450	-0.000000
O1_4	0.000000	0.018450	-0.000000
O1_5	0.000000	0.000000	0.000000
O1_6	0.000000	0.000000	0.000000

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 230 Ia-3d Oh-10

Transformation matrix:

```
[       1       0       0  ] [         0]
[       0       1       0  ] [         0]
[       0       0       1  ] [         0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.4060 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

T1 1	O1 1	O1 2	O1 3
-0.1464	0.0116	-0.7052	0.6936

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:

(normalization unit: 1 Ångström)

Atom	δx	δy	δz
K1	0.0000	0.0000	0.0000
T1	0.0016	-0.0000	-0.0016
T1_2	-0.0016	0.0000	0.0016
T1_3	-0.0016	0.0016	-0.0000
O1	0.0001	-0.0075	0.0074
O1_2	-0.0001	-0.0075	-0.0074
O1_3	0.0074	0.0001	-0.0075
O1_4	0.0074	-0.0001	0.0075
O1_5	-0.0075	0.0074	0.0001
O1_6	0.0075	0.0074	-0.0001

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM3+

Direction: (a,0)

Isotropy Subgroup: 142 I4_1/acd D4h-20

Transformation matrix:

```
[       1       0       0  ] [         0]
[       0       1       0  ] [         0]
[       0       0       1  ] [         0]
```

The amplitude of this distortion is:
A_{GM3+}= 1.7219 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

K1 1	T1 1	T1 2	T1 3	O1 1	O1 2	O1 3	O1 4	O1 5	O1 6
-0.0142	0.3168	0.0367	0.0535	-0.3662	0.6076	0.4588	0.3361	-0.0540	-0.2560

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:
(normalization unit: 1 Ångström)

Atom	δx	δy	δz
K1	0.0003	-0.0003	0.0000
T1	-0.0029	0.0010	0.0019
T1_2	0.0029	0.0010	-0.0019
T1_3	-0.0048	0.0048	-0.0000
O1	-0.0008	0.0069	-0.0055
O1_2	0.0008	0.0069	0.0055
O1_3	-0.0006	0.0083	0.0009
O1_4	-0.0006	-0.0083	-0.0009
O1_5	-0.0078	0.0061	-0.0075
O1_6	0.0078	0.0061	0.0075

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM4+

Direction: (0,0,a)

Isotropy Subgroup: 88 I4_1/a C4h-6

Transformation matrix:

```
[      1      0      0 ] [     1/2]
[      0      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{GM4+}= 4.5374 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

K1 1	K1 2	T1 1	T1 2	T1 3	T1 4	T1 5	O1 1	O1 2	O1 3	O1 4	O1 5	O1 6	O1 7	O1 8	O1 9
0.0507	-0.1176	-0.2234	0.1846	0.0253	0.2389	0.2091	0.4742	-0.0759	-0.4778	0.0131	0.1648	-0.0102	0.2849	0.2968	0.3775

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure: (normalization unit: 1 Ångström)

Atom	δx	δy	δz
K1	-0.0020	-0.0020	-0.0017
T1	-0.0056	0.0044	0.0002
T1_2	-0.0056	-0.0044	0.0002
T1_3	0.0034	0.0034	-0.0007
O1	-0.0002	0.0053	0.0030
O1_2	-0.0002	-0.0053	0.0030
O1_3	0.0088	0.0070	-0.0014
O1_4	-0.0088	0.0070	-0.0014
O1_5	0.0055	-0.0088	0.0002
O1_6	0.0055	0.0088	0.0002

Virtual structure with only this symmetry component of the distortion frozen.

KNiCl3- (Visser et al. Acta Crystallographica B (1980) 36, 28)

Symmetry mode analysis

High symmetry structure

```
194
6.80985 6.80985 5.926 90 90 120
3
Ni      1       2a      0.000000        0.000000        0.000000
K       1       2d      0.333333        0.666667        0.750000
Cl      1       6h      0.160000        0.320000        0.250000
```

Low symmetry structure

```
185
11.795 11.795 5.926 90 90 120
5
K       1       6c      0.335300        0.335300        0.329400
Ni      1       2a      0.000000        0.000000        0.000000
Ni      2       4b      0.333333        0.666667        0.123000
Cl      1       6c      0.159800        0.000000        0.260400
Cl      2       12d     0.505600        0.173200        0.385200
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
11.795007 11.795007 5.926000 90.000000 90.000000 120.000000
5
Ni      1       2a      0.000000        0.000000        0.000000
Ni      1_2     4b      0.666667        0.333333        0.000000
K       1       6c      0.333334        0.000000        0.750000
Cl      1       6c      0.160000        0.000000        0.250000
Cl      1_2     12d     0.826667        0.333333        0.250000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Ni1	(0.000000,0.000000,0.000000)	Ni1	(0.000000,0.000000,0.000000)
4b	(1/3,2/3,z)	Ni1_2	(0.666667,0.333333,0.000000)	Ni2	(0.666667,0.333333,0.123000)

6c	(x,0,z)	K1	(0.333334,0.000000,0.750000)	K1	(0.335300,0.000000,0.829400)
6c	(x,0,z)	Cl1	(0.160000,0.000000,0.250000)	Cl1	(0.159800,0.000000,0.260400)
12d	(x,y,z)	Cl1_2	(0.826667,0.333333,0.250000)	Cl2	(0.826800,0.332400,0.385200)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ni1	0.0000	0.0000	0.0000	0.0000
4b	(1/3,2/3,z)	Ni1_2	0.0000	0.0000	0.1230	0.7289
6c	(x,0,z)	K1	0.0020	0.0000	0.0794	0.4711
6c	(x,0,z)	Cl1	-0.0002	0.0000	0.0104	0.0617
12d	(x,y,z)	Cl1_2	0.0001	-0.0009	0.1352	0.8013

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.8013 Å
Total distortion amplitude: 3.3443 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.08844)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Ni1	(0.000000,0.000000,0.000000)	Ni1	(0.000000,0.000000,0.911560)
4b	(1/3,2/3,z)	Ni1_2	(0.666667,0.333333,0.000000)	Ni2	(0.666667,0.333333,0.034560)
6c	(x,0,z)	K1	(0.333334,0.000000,0.750000)	K1	(0.335300,0.000000,0.740960)
6c	(x,0,z)	Cl1	(0.160000,0.000000,0.250000)	Cl1	(0.159800,0.000000,0.171960)
12d	(x,y,z)	Cl1_2	(0.826667,0.333333,0.250000)	Cl2	(0.826800,0.332400,0.296760)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ni1	0.0000	0.0000	-0.0884	0.5241
4b	(1/3,2/3,z)	Ni1_2	0.0000	0.0000	0.0346	0.2048
6c	(x,0,z)	K1	0.0020	0.0000	-0.0090	0.0584
6c	(x,0,z)	Cl1	-0.0002	0.0000	-0.0780	0.4625

12d	(x,y,z)	Cl1_2	0.0001	-0.0009	0.0468	0.2774

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.5241 Å
Total distortion amplitude: 1.7159 Å

Symmetry Modes Summary

Atoms	WP	Modes
Cl1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
K1	2*d*	GM2-(1) K1(1)
Ni1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.0167
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.2069
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.0684
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	1.7018

Global distortion: 1.7158 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.019983	-0.000000	-0.000000
Cl1_2	0.019983	-0.000000	-0.000000

Irrep GM2-

GM2- Mode Ni1 1

Atom	δx	δy	δz
Ni1	0.000000	0.000000	0.068891
Ni1_2	0.000000	0.000000	0.068891

GM2- Mode K1 1

Atom	δx	δy	δz
K1	0.000000	0.000000	0.068891

GM2- Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.039774
Cl1_2	0.000000	0.000000	0.039774

Irrep K1

K1 Mode K1 1

Atom	δx	δy	δz
K1	0.034612	-0.000000	-0.000000

K1 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.000000
Cl1_2	-0.014130	-0.028261	0.000000

K1 Mode Cl1 2

Atom	δx	δy	δz
Cl1	0.028261	-0.000000	-0.000000
Cl1_2	-0.014130	0.000000	0.000000

Irrep K3

K3 Mode Ni1 1

Atom	δx	δy	δz
Ni1	0.000000	0.000000	0.097427
Ni1_2	0.000000	0.000000	-0.048713

K3 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.056249
Cl1_2	0.000000	0.000000	-0.028125

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.0167 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Cl1 1
0.0167

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ni1	0.0000	0.0000	0.0000
Ni1_2	0.0000	0.0000	0.0000
K1	0.0000	0.0000	0.0000
Cl1	0.0200	-0.0000	-0.0000
Cl1_2	0.0200	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM2-} = 0.2069 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ni1 1	K1 1	Cl1 1
-0.4519	-0.6344	0.6272

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ni1	0.0000	0.0000	-0.0311
Ni1_2	0.0000	0.0000	-0.0311
K1	0.0000	0.0000	-0.0437
Cl1	0.0000	0.0000	0.0249
Cl1_2	0.0000	0.0000	0.0249

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K1}= 0.0684 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

K1 1	Cl1 1	Cl1 2
0.8310	0.4830	-0.2759

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ni1	0.0000	0.0000	0.0000
Ni1_2	0.0000	0.0000	0.0000
K1	0.0288	-0.0000	-0.0000
Cl1	-0.0078	0.0000	0.0000
Cl1_2	-0.0029	-0.0137	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{K3}= 1.7018 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ni1 1	Cl1 1
-0.4946	-0.8691

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ni1	0.0000	0.0000	-0.0482
Ni1_2	0.0000	0.0000	0.0241
K1	0.0000	0.0000	0.0000
Cl1	0.0000	0.0000	-0.0489
Cl1_2	0.0000	0.0000	0.0244

Virtual structure with only this symmetry component of the distortion frozen.

TlFeBr3-(Jouini et al. Materials Research Bulletin (1982) 17, 1421)

Symmetry mode analysis

High symmetry structure

```
194
7.18455 7.18455 6.23 90 90 120
3
Fe      1       2a      0.000000        0.000000        0.000000
Tl      1       2d      0.333333        0.666667        0.750000
Br      1       6h      0.160000        0.320000        0.250000
```

Low symmetry structure

```
185
12.444 12.444 6.23 90 90 120
5
Tl      1       6c      0.336000        0.000000        0.250000
Fe      1       2a      0.000000        0.000000        0.052000
Fe      2       4b      0.333333        0.666667        -0.030000
Br      1       6c      0.839000        0.000000        0.323000
Br      2       12d     0.169800        0.666000        0.244000
```

Transformation matrix

```
[     1    -2     0 ] [       0]
[     2    -1     0 ] [       0]
[     0     0     1 ] [0.45000]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
12.444005 12.444005 6.230000 90.000000 90.000000 120.000000
5
Fe      1       2a      0.000000        0.000000        0.550000
Fe      1_2     4b      0.666667        0.333333        0.550000
Tl      1       6c      0.333334        0.000000        0.300000
Br      1       6c      0.160000        0.000000        0.800000
Br      1_2     12d     0.826667        0.333333        0.800000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
2a	(0,0,z)	Fe1	(0.000000,0.000000,0.550000)	Fe1	(0.000000,0.000000,0.552000)

4b	(1/3,2/3,z)	Fe1_2	(0.666667,0.333333,0.550000)	Fe2	(0.666667,0.333333,0.470000)
6c	(x,0,z)	Tl1	(0.333334,0.000000,0.300000)	Tl1	(0.336000,0.000000,0.250000)
6c	(x,0,z)	Br1	(0.160000,0.000000,0.800000)	Br1	(0.161000,0.000000,0.823000)
12d	(x,y,z)	Br1_2	(0.826667,0.333333,0.800000)	Br2	(0.830200,0.334000,0.744000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Fe1	0.0000	0.0000	0.0020	0.0125
4b	(1/3,2/3,z)	Fe1_2	0.0000	0.0000	-0.0800	0.4984
6c	(x,0,z)	Tl1	0.0027	0.0000	-0.0500	0.3133
6c	(x,0,z)	Br1	0.0010	0.0000	0.0230	0.1438
12d	(x,y,z)	Br1_2	0.0035	0.0007	-0.0560	0.3512

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4984 Å
Total distortion amplitude: 1.7852 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.03833)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Fe1	(0.000000,0.000000,0.550000)	Fe1	(0.000000,0.000000,0.590333)
4b	(1/3,2/3,z)	Fe1_2	(0.666667,0.333333,0.550000)	Fe2	(0.666667,0.333333,0.508333)
6c	(x,0,z)	Tl1	(0.333334,0.000000,0.300000)	Tl1	(0.336000,0.000000,0.288333)
6c	(x,0,z)	Br1	(0.160000,0.000000,0.800000)	Br1	(0.161000,0.000000,0.861333)
12d	(x,y,z)	Br1_2	(0.826667,0.333333,0.800000)	Br2	(0.830200,0.334000,0.782333)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Fe1	0.0000	0.0000	0.0403	0.2513
4b	(1/3,2/3,z)	Fe1_2	0.0000	0.0000	-0.0417	0.2596
6c	(x,0,z)	Tl1	0.0027	0.0000	-0.0117	0.0799

6c	(x,0,z)	Br1	0.0010	0.0000	0.0613	0.3823
12d	(x,y,z)	Br1_2	0.0035	0.0007	-0.0177	0.1173

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.3823 Å
Total distortion amplitude: 1.2150 Å

Symmetry Modes Summary

Atoms	WP	Modes
Br1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
Tl1	2*d*	GM2-(1) K1(1)
Fe1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.1302
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.3633
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.1011
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	1.1476

Global distortion: 1.2149 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Br1 1

Atom	δx	δy	δz
Br1	0.018941	0.000000	-0.000000
Br1_2	0.018941	0.000000	-0.000000

Irrep GM2-

GM2- Mode Fe1 1

Atom	δx	δy	δz
Fe1	0.000000	0.000000	0.065529
Fe1_2	0.000000	0.000000	0.065529

GM2- Mode Tl1 1

Atom	δx	δy	δz
Tl1	0.000000	0.000000	0.065529

GM2- Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.037833
Br1_2	0.000000	0.000000	0.037833

Irrep K1

K1 Mode Tl1 1

Atom	δx	δy	δz
Tl1	0.032807	0.000000	-0.000000

K1 Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.000000
Br1_2	-0.013393	-0.026787	0.000000

K1 Mode Br1 2

Atom	δx	δy	δz
Br1	0.026787	0.000000	-0.000000
Br1_2	-0.013393	0.000000	0.000000

Irrep K3

K3 Mode Fe1 1

Atom	δx	δy	δz
Fe1	0.000000	0.000000	0.092673
Fe1_2	0.000000	0.000000	-0.046336

K3 Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.053505
Br1_2	0.000000	0.000000	-0.026752

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.1302 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Br1 1
0.1302

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Fe1	0.0000	0.0000	0.0000
Fe1_2	0.0000	0.0000	0.0000
Tl1	0.0000	0.0000	0.0000
Br1	0.0189	0.0000	-0.0000
Br1_2	0.0189	0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM2-} = 0.3633 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Fe1 1	Tl1 1	Br1 1
-0.6020	-0.4900	0.6304

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Fe1	0.0000	0.0000	-0.0394
Fe1_2	0.0000	0.0000	-0.0394
Tl1	0.0000	0.0000	-0.0321
Br1	0.0000	0.0000	0.0239

Br1_2	0.0000	0.0000	0.0239

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K1} = 0.1011 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Tl1 1	Br1 1	Br1 2
0.8038	-0.2463	-0.5415

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Fe1	0.0000	0.0000	0.0000
Fe1_2	0.0000	0.0000	0.0000
Tl1	0.0264	0.0000	-0.0000
Br1	-0.0145	-0.0000	0.0000
Br1_2	0.0106	0.0066	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [0.45000]
```

The amplitude of this distortion is:
A_{K3}= 1.1476 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Fe1 1	Br1 1
0.5140	0.8578

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Fe1	0.0000	0.0000	0.0476
Fe1_2	0.0000	0.0000	-0.0238
Tl1	0.0000	0.0000	0.0000
Br1	0.0000	0.0000	0.0459
Br1_2	0.0000	0.0000	-0.0229

Virtual structure with only this symmetry component of the distortion frozen.

RbMnBr3-(Fink, H.;Seifert, H.J., Acta Crystallographica B (1982) 38, 912-914)

Symmetry mode analysis

High symmetry structure

```
194
7.46167 7.46167 6.796 90 90 120
3
Mn      1       2a      0.000000        0.000000        0.000000
Rb      1       2d      0.333333        0.666667        0.750000
Br      1       6h      0.160000        0.320000        0.250000
```

Low symmetry structure

```
185
12.9240 12.9240 6.5470 90.00 90.00 120.00
5
Rb      1       6c      0.334000        0.000000        0.298500
Mn      1       2a      0.000000        0.000000        0.000000
Mn      2       4b      0.333333        0.666667        0.108800
Br      1       6c      0.837000        0.000000        0.251700
Br      2       12d     0.333500        0.503700        0.361500
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [0.45000]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
12.923991 12.923991 6.796000 90.000000 90.000000 120.000000
5
Mn      1       2a      0.000000        0.000000        0.550000
Mn      1_2     4b      0.666667        0.333333        0.550000
Rb      1       6c      0.333334        0.000000        0.300000
Br      1       6c      0.160000        0.000000        0.800000
Br      1_2     12d     0.826667        0.333333        0.800000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.550000)	Mn1	(0.000000,0.000000,0.500000)

4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.550000)	Mn2	(0.666667,0.333333,0.608800)
6c	(x,0,z)	Rb1	(0.333334,0.000000,0.300000)	Rb1	(0.334000,0.000000,0.298500)
6c	(x,0,z)	Br1	(0.160000,0.000000,0.800000)	Br1	(0.163000,0.000000,0.751700)
12d	(x,y,z)	Br1_2	(0.826667,0.333333,0.800000)	Br2	(0.829800,0.333500,0.861500)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	-0.0500	0.3398
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	0.0588	0.3996
6c	(x,0,z)	Rb1	0.0007	0.0000	-0.0015	0.0133
6c	(x,0,z)	Br1	0.0030	0.0000	-0.0483	0.3305
12d	(x,y,z)	Br1_2	0.0031	0.0002	0.0615	0.4198

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4198 Å
Total distortion amplitude: 1.9081 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.01915)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.550000)	Mn1	(0.000000,0.000000,0.480853)
4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.550000)	Mn2	(0.666667,0.333333,0.589653)
6c	(x,0,z)	Rb1	(0.333334,0.000000,0.300000)	Rb1	(0.334000,0.000000,0.279353)
6c	(x,0,z)	Br1	(0.160000,0.000000,0.800000)	Br1	(0.163000,0.000000,0.732553)
12d	(x,y,z)	Br1_2	(0.826667,0.333333,0.800000)	Br2	(0.829800,0.333500,0.842353)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	-0.0691	0.4699
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	0.0397	0.2695
6c	(x,0,z)	Rb1	0.0007	0.0000	-0.0206	0.1406

6c	(x,0,z)	Br1	0.0030	0.0000	-0.0674	0.4600
12d	(x,y,z)	Br1_2	0.0031	0.0002	0.0424	0.2905

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4699 Å
Total distortion amplitude: 1.7700 Å

Symmetry Modes Summary

Atoms	WP	Modes
Br1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
Rb1	2*d*	GM2-(1) K1(1)
Mn1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.1663
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.3858
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.0221
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	1.7194

Global distortion: 1.7701 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Br1 1

Atom	δx	δy	δz
Br1	0.018238	-0.000000	-0.000000
Br1_2	0.018238	-0.000000	-0.000000

Irrep GM2-

GM2- Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.060072
Mn1_2	0.000000	0.000000	0.060072

GM2- Mode Rb1 1

Atom	δx	δy	δz
Rb1	0.000000	0.000000	0.060072

GM2- Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.034682
Br1_2	0.000000	0.000000	0.034682

Irrep K1

K1 Mode Rb1 1

Atom	δx	δy	δz
Rb1	0.031588	-0.000000	-0.000000

K1 Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.000000
Br1_2	-0.012896	-0.025792	0.000000

K1 Mode Br1 2

Atom	δx	δy	δz
Br1	0.025792	-0.000000	-0.000000
Br1_2	-0.012896	0.000000	0.000000

Irrep K3

K3 Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.084954
Mn1_2	0.000000	0.000000	-0.042477

K3 Mode Br1 1

Atom	δx	δy	δz
Br1	0.000000	0.000000	0.049048
Br1_2	0.000000	0.000000	-0.024524

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.1663 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Br1 1
0.1663

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Rb1	0.0000	0.0000	0.0000
Br1	0.0182	-0.0000	-0.0000
Br1_2	0.0182	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM2-} = 0.3858 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	Rb1 1	Br1 1
0.1461	-0.8909	0.4300

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0088
Mn1_2	0.0000	0.0000	0.0088
Rb1	0.0000	0.0000	-0.0535
Br1	0.0000	0.0000	0.0149

Br1_2	0.0000	0.0000	0.0149

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K1}= 0.0221 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Rb1 1	Br1 1	Br1 2
0.9543	-0.2931	-0.0579

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Rb1	0.0301	-0.0000	-0.0000
Br1	-0.0015	0.0000	0.0000
Br1_2	0.0045	0.0076	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [0.45000]
```

The amplitude of this distortion is:
A_{K3}= 1.7194 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	Br1 1
-0.4966	-0.8680

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	-0.0422
Mn1_2	0.0000	0.0000	0.0211
Rb1	0.0000	0.0000	0.0000
Br1	0.0000	0.0000	-0.0426
Br1_2	0.0000	0.0000	0.0213

Virtual structure with only this symmetry component of the distortion frozen.

BaMnO3-80K (Cussen, E.J.;Battle, P.D., Chemistry of Materials (2000) 12, 831-838)

Symmetry mode analysis

High symmetry structure

```
194
5.68499 5.68499 4.8075 90 90 120
3
Mn       1        2a       0.000000         0.000000         0.000000
Ba       1        2d       0.333333         0.666667         0.750000
O        1        6h       0.150333         0.300666         0.250000
```

Low symmetry structure

```
185
9.8467 9.8467 4.8075 90.00 90.00 120.00
5
Ba       1        6c       0.332000         0.332000         0.238000
Mn       1        2a       0.000000         0.000000         0.000000
Mn       2        4b       0.666667         0.333333         0.963000
O        1        6c       0.000000         0.150000         0.250000
O        2        12d      0.667000         0.484000         0.212000
```

Transformation matrix

```
[      1     -2      0  ] [       0]
[      2     -1      0  ] [       0]
[      0      0      1  ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
9.846692 9.846692 4.807500 90.000000 90.000000 120.000000
5
Mn       1        2a       0.000000         0.000000         0.000000
Mn       1_2      4b       0.666667         0.333333         0.000000
Ba       1        6c       0.333334         0.000000         0.750000
O        1        6c       0.150333         0.000000         0.250000
O        1_2      12d      0.817000         0.333333         0.250000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.000000)	Mn1	(0.000000,0.000000,0.000000)

4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.000000)	Mn2	(0.666667,0.333333,0.963000)
6c	(x,0,z)	Ba1	(0.333334,0.000000,0.750000)	Ba1	(0.332000,0.000000,0.738000)
6c	(x,0,z)	O1	(0.150333,0.000000,0.250000)	O1	(0.150000,0.000000,0.250000)
12d	(x,y,z)	O1_2	(0.817000,0.333333,0.250000)	O2	(0.817000,0.333000,0.212000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	0.0000	0.0000
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	-0.0370	0.1779
6c	(x,0,z)	Ba1	-0.0013	0.0000	-0.0120	0.0592
6c	(x,0,z)	O1	-0.0003	0.0000	0.0000	0.0033
12d	(x,y,z)	O1_2	0.0000	-0.0003	-0.0380	0.1827

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1827 Å
Total distortion amplitude: 0.7404 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.02253)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.000000)	Mn1	(0.000000,0.000000,0.022533)
4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.000000)	Mn2	(0.666667,0.333333,0.985533)
6c	(x,0,z)	Ba1	(0.333334,0.000000,0.750000)	Ba1	(0.332000,0.000000,0.760533)
6c	(x,0,z)	O1	(0.150333,0.000000,0.250000)	O1	(0.150000,0.000000,0.272533)
12d	(x,y,z)	O1_2	(0.817000,0.333333,0.250000)	O2	(0.817000,0.333000,0.234533)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	0.0225	0.1083
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	-0.0145	0.0696
6c	(x,0,z)	Ba1	-0.0013	0.0000	0.0105	0.0523

6c	(x,0,z)	O1	-0.0003	0.0000	0.0225	0.1084
12d	(x,y,z)	O1_2	0.0000	-0.0003	-0.0155	0.0744

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1084 Å
Total distortion amplitude: 0.4429 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
Ba1	2*d*	GM2-(1) K1(1)
Mn1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.0000
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.1388
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.0351
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	0.4191

Global distortion: 0.4429 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode O1 1

Atom	δx	δy	δz
O1	0.023937	0.000000	-0.000000
O1_2	0.023937	0.000000	-0.000000

Irrep GM2-

GM2- Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.084919
Mn1_2	0.000000	0.000000	0.084919

GM2- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.084919

GM2- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.049028
O1_2	0.000000	0.000000	0.049028

Irrep K1

K1 Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.041460	0.000000	-0.000000

K1 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	-0.016926	-0.033852	0.000000

K1 Mode O1 2

Atom	δx	δy	δz
O1	0.033852	0.000000	-0.000000
O1_2	-0.016926	0.000000	0.000000

Irrep K3

K3 Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.120094
Mn1_2	0.000000	0.000000	-0.060047

K3 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.069336
O1_2	0.000000	0.000000	-0.034668

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[       1       0       0 ] [       0]
[       0       1       0 ] [       0]
[       0       0       1 ] [       0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.0000 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O1 1
-0.0000

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Ba1	0.0000	0.0000	0.0000
O1	-0.0239	-0.0000	0.0000
O1_2	-0.0239	-0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM2-} = 0.1388 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	Ba1 1	O1 1
-0.1810	0.8933	-0.4114

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	-0.0154
Mn1_2	0.0000	0.0000	-0.0154
Ba1	0.0000	0.0000	0.0759
O1	0.0000	0.0000	-0.0202

O1_2	0.0000	0.0000	-0.0202

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0  ] [       0]
[      1      1      0  ] [       0]
[      0      0      1  ] [       0]
```

The amplitude of this distortion is:
A_{K1}= 0.0351 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ba1 1	O1 1	O1 2
-0.9179	0.2806	-0.2806

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Ba1	-0.0381	-0.0000	0.0000
O1	-0.0095	-0.0000	0.0000
O1_2	0.0000	-0.0095	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [      0]
[      2     -1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K3}= 0.4191 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	O1 1
0.4900	0.8717

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0588
Mn1_2	0.0000	0.0000	-0.0294
Ba1	0.0000	0.0000	0.0000
O1	0.0000	0.0000	0.0604
O1_2	0.0000	0.0000	-0.0302

Virtual structure with only this symmetry component of the distortion frozen.

BaMnO3-1.7K (Cussen, E.J.;Battle, P.D., Chemistry of Materials (2000) 12, 831-838)

Symmetry mode analysis

High symmetry structure

```
194
5.68499 5.68499 4.8075 90 90 120
3
Mn       1        2a       0.000000         0.000000         0.000000
Ba       1        2d       0.333333         0.666667         0.750000
O        1        6h       0.150333         0.300666         0.250000
```

Low symmetry structure

```
185
9.8467 9.8467 4.8075 90.00 90.00 120.00
5
Ba       1        6c       0.339000         0.339000         0.230000
Mn       1        2a       0.000000         0.000000         0.000000
Mn       2        4b       0.666667         0.333333         0.952000
O        1        6c       0.000000         0.149200         0.248000
O        2        12d      0.664400         0.482400         0.200000
```

Transformation matrix

```
[      1     -2      0  ] [       0]
[      2     -1      0  ] [       0]
[      0      0      1  ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
9.846692 9.846692 4.807500 90.000000 90.000000 120.000000
5
Mn       1        2a       0.000000         0.000000         0.000000
Mn       1_2      4b       0.666667         0.333333         0.000000
Ba       1        6c       0.333334         0.000000         0.750000
O        1        6c       0.150333         0.000000         0.250000
O        1_2      12d      0.817000         0.333333         0.250000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.000000)	Mn1	(0.000000,0.000000,0.000000)

4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.000000)	Mn2	(0.666667,0.333333,0.952000)
6c	(x,0,z)	Ba1	(0.333334,0.000000,0.750000)	Ba1	(0.339000,0.000000,0.730000)
6c	(x,0,z)	O1	(0.150333,0.000000,0.250000)	O1	(0.149200,0.000000,0.248000)
12d	(x,y,z)	O1_2	(0.817000,0.333333,0.250000)	O2	(0.818000,0.335600,0.200000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	0.0000	0.0000
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	-0.0480	0.2308
6c	(x,0,z)	Ba1	0.0057	0.0000	-0.0200	0.1112
6c	(x,0,z)	O1	-0.0011	0.0000	-0.0020	0.0147
12d	(x,y,z)	O1_2	0.0010	0.0023	-0.0500	0.2412

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2412 Å
Total distortion amplitude: 0.9933 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.03080)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Mn1	(0.000000,0.000000,0.000000)	Mn1	(0.000000,0.000000,0.030800)
4b	(1/3,2/3,z)	Mn1_2	(0.666667,0.333333,0.000000)	Mn2	(0.666667,0.333333,0.982800)
6c	(x,0,z)	Ba1	(0.333334,0.000000,0.750000)	Ba1	(0.339000,0.000000,0.760800)
6c	(x,0,z)	O1	(0.150333,0.000000,0.250000)	O1	(0.149200,0.000000,0.278800)
12d	(x,y,z)	O1_2	(0.817000,0.333333,0.250000)	O2	(0.818000,0.335600,0.230800)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Mn1	0.0000	0.0000	0.0308	0.1481
4b	(1/3,2/3,z)	Mn1_2	0.0000	0.0000	-0.0172	0.0827
6c	(x,0,z)	Ba1	0.0057	0.0000	0.0108	0.0762

6c	(x,0,z)	O1	-0.0011	0.0000	0.0288	0.1389
12d	(x,y,z)	O1_2	0.0010	0.0023	-0.0192	0.0943

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1481 Å
Total distortion amplitude: 0.5732 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
Ba1	2*d*	GM2-(1) K1(1)
Mn1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.0195
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.1436
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.1535
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	0.5329

Global distortion: 0.5732 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode O1 1

Atom	δx	δy	δz
O1	0.023937	0.000000	-0.000000
O1_2	0.023937	0.000000	-0.000000

Irrep GM2-

GM2- Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.084919
Mn1_2	0.000000	0.000000	0.084919

GM2- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.084919

GM2- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.049028
O1_2	0.000000	0.000000	0.049028

Irrep K1

K1 Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.041460	0.000000	-0.000000

K1 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	-0.016926	-0.033852	0.000000

K1 Mode O1 2

Atom	δx	δy	δz
O1	0.033852	0.000000	-0.000000
O1_2	-0.016926	0.000000	0.000000

Irrep K3

K3 Mode Mn1 1

Atom	δx	δy	δz
Mn1	0.000000	0.000000	0.120094
Mn1_2	0.000000	0.000000	-0.060047

K3 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.000000	0.069336
O1_2	0.000000	0.000000	-0.034668

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[       1       0       0 ] [       0]
[       0       1       0 ] [       0]
[       0       0       1 ] [       0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.0195 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O1 1
-0.0195

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Ba1	0.0000	0.0000	0.0000
O1	-0.0239	-0.0000	0.0000
O1_2	-0.0239	-0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[       1       0       0 ] [       0]
[       0       1       0 ] [       0]
[       0       0       1 ] [       0]
```

The amplitude of this distortion is:
$A_{GM2-} = 0.1436$ Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	Ba1 1	O1 1
-0.0984	0.8854	-0.4544

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	-0.0084
Mn1_2	0.0000	0.0000	-0.0084
Ba1	0.0000	0.0000	0.0752
O1	0.0000	0.0000	-0.0223

O1_2	0.0000	0.0000	-0.0223

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0  ] [       0]
[      1      1      0  ] [       0]
[      0      0      1  ] [       0]
```

The amplitude of this distortion is:
A_{K1}= 0.1535 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ba1 1	O1 1	O1 2
0.8906	-0.4364	-0.1283

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
Mn1_2	0.0000	0.0000	0.0000
Ba1	0.0369	0.0000	-0.0000
O1	-0.0043	-0.0000	0.0000
O1_2	0.0096	0.0148	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [      0]
[      2     -1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K3}= 0.5329 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Mn1 1	O1 1
0.5000	0.8660

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0600
Mn1_2	0.0000	0.0000	-0.0300
Ba1	0.0000	0.0000	0.0000
O1	0.0000	0.0000	0.0600
O1_2	0.0000	0.0000	-0.0300

Virtual structure with only this symmetry component of the distortion frozen.

TlCoCl3 (Nishiwaki et al., J. Phys. Soc. Japan (2006) 75, 034707)

Symmetry mode analysis

High symmetry structure

```
194
6.84737 6.84737 5.98 90 90 120
3
Co      1       2a      0.000000        0.000000        0.000000
Tl      1       2d      0.333333        0.666667        0.750000
Cl      1       6h      0.160000        0.320000        0.250000
```

Low symmetry structure

```
185
11.86 11.86 5.98 90 90 120
5
Tl      1       6c      0.666800        0.000000        0.250000
Co      1       2a      0.000000        0.000000        -0.037400
Co      2       4b      0.333333        0.666667        0.037200
Cl      1       6c      0.163000        0.000000        0.213100
Cl      2       12d     0.333500        0.829700        0.286600
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
185
11.859993 11.859993 5.980000 90.000000 90.000000 120.000000
5
Co      1       2a      0.000000        0.000000        0.000000
Co      1_2     4b      0.666667        0.333333        0.000000
Tl      1       6c      0.333334        0.000000        0.750000
Cl      1       6c      0.160000        0.000000        0.250000
Cl      1_2     12d     0.826667        0.333333        0.250000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Co1	(0.000000,0.000000,0.000000)	Co1	(0.000000,0.000000,0.962600)

4b	(1/3,2/3,z)	Co1_2	(0.666667,0.333333,0.000000)	Co2	(0.666667,0.333333,0.037200)
6c	(x,0,z)	Tl1	(0.333334,0.000000,0.750000)	Tl1	(0.333200,0.000000,0.750000)
6c	(x,0,z)	Cl1	(0.160000,0.000000,0.250000)	Cl1	(0.163000,0.000000,0.213100)
12d	(x,y,z)	Cl1_2	(0.826667,0.333333,0.250000)	Cl2	(0.829700,0.333500,0.286600)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Co1	0.0000	0.0000	-0.0374	0.2237
4b	(1/3,2/3,z)	Co1_2	0.0000	0.0000	0.0372	0.2225
6c	(x,0,z)	Tl1	-0.0001	0.0000	0.0000	0.0016
6c	(x,0,z)	Cl1	0.0030	0.0000	-0.0369	0.2235
12d	(x,y,z)	Cl1_2	0.0030	0.0002	0.0366	0.2217

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2237 Å
Total distortion amplitude: 1.0898 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.00973)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Co1	(0.000000,0.000000,0.000000)	Co1	(0.000000,0.000000,0.952873)
4b	(1/3,2/3,z)	Co1_2	(0.666667,0.333333,0.000000)	Co2	(0.666667,0.333333,0.027473)
6c	(x,0,z)	Tl1	(0.333334,0.000000,0.750000)	Tl1	(0.333200,0.000000,0.740273)
6c	(x,0,z)	Cl1	(0.160000,0.000000,0.250000)	Cl1	(0.163000,0.000000,0.203373)
12d	(x,y,z)	Cl1_2	(0.826667,0.333333,0.250000)	Cl2	(0.829700,0.333500,0.276873)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Co1	0.0000	0.0000	-0.0471	0.2818
4b	(1/3,2/3,z)	Co1_2	0.0000	0.0000	0.0275	0.1643
6c	(x,0,z)	Tl1	-0.0001	0.0000	-0.0097	0.0582

6c	(x,0,z)	Cl1	0.0030	0.0000	-0.0466	0.2811
12d	(x,y,z)	Cl1_2	0.0030	0.0002	0.0269	0.1645

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2818 Å
Total distortion amplitude: 1.0421 Å

Symmetry Modes Summary

Atoms	WP	Modes
Cl1	6*h*	GM1+(1) GM2-(1) K1(2) **K3(1)**
Tl1	2*d*	GM2-(1) K1(1)
Co1	2*a*	GM2-(1) **K3(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.1493
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.1593
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.0072
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	1.0189

Global distortion: 1.0420 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.019874	0.000000	-0.000000
Cl1_2	0.019874	0.000000	-0.000000

Irrep GM2-

GM2- Mode Co1 1

Atom	δx	δy	δz
Co1	0.000000	0.000000	0.068269
Co1_2	0.000000	0.000000	0.068269

GM2- Mode Tl1 1

Atom	δx	δy	δz
Tl1	0.000000	0.000000	0.068269

GM2- Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.039415
Cl1_2	0.000000	0.000000	0.039415

Irrep K1

K1 Mode Tl1 1

Atom	δx	δy	δz
Tl1	0.034422	0.000000	-0.000000

K1 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.000000
Cl1_2	-0.014053	-0.028106	0.000000

K1 Mode Cl1 2

Atom	δx	δy	δz
Cl1	0.028106	0.000000	-0.000000
Cl1_2	-0.014053	-0.000000	0.000000

Irrep K3

K3 Mode Co1 1

Atom	δx	δy	δz
Co1	0.000000	0.000000	0.096547
Co1_2	0.000000	0.000000	-0.048273

K3 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.055741
Cl1_2	0.000000	0.000000	-0.027871

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[       1       0       0 ] [       0]
[       0       1       0 ] [       0]
[       0       0       1 ] [       0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.1493 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Cl1 1
0.1493

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Co1	0.0000	0.0000	0.0000
Co1_2	0.0000	0.0000	0.0000
Tl1	0.0000	0.0000	0.0000
Cl1	0.0199	0.0000	-0.0000
Cl1_2	0.0199	0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
$A_{GM2-} = 0.1593$ Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Co1 1	Tl1 1	Cl1 1
0.2396	-0.8943	0.3779

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Co1	0.0000	0.0000	0.0164
Co1_2	0.0000	0.0000	0.0164
Tl1	0.0000	0.0000	-0.0611
Cl1	0.0000	0.0000	0.0149

Cl1_2	0.0000	0.0000	0.0149

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K1}= 0.0072 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Tl1 1	Cl1 1	Cl1 2
-0.5404	-0.8248	0.1663

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Co1	0.0000	0.0000	0.0000
Co1_2	0.0000	0.0000	0.0000
Tl1	-0.0186	-0.0000	0.0000
Cl1	0.0047	0.0000	-0.0000
Cl1_2	0.0093	0.0232	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{K3}= 1.0189 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Co1 1	Cl1 1
-0.5056	-0.8628

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Co1	0.0000	0.0000	-0.0488
Co1_2	0.0000	0.0000	0.0244
Tl1	0.0000	0.0000	0.0000
Cl1	0.0000	0.0000	-0.0481
Cl1_2	0.0000	0.0000	0.0240

Virtual structure with only this symmetry component of the distortion frozen.

KTiCL3

ref: Liesbet Jongen, Thomas Gloger, Jan Beekhuizen, and Gerd Meyer Z. Anorg. Allg. Chem. 2005, 631, 582_586. virtual high symmetry cell with no strain

Symmetry mode analysis

High symmetry structure

```
194
7.00615 7.00615 6.055 90 90 120
3
Ti     1    2a     0.0 0.0 0.0
K      1    2d     0.333333 0.666667 0.75
Cl     1    6h     0.16 0.32 0.25
```

Low symmetry structure

```
173
12.1350 12.1350 6.0550 90.00 90.00 120.00
7
K      1    6c     0.004 0.341 0.180
Ti     1    2a     0.0 0.0 0.028
Ti     2    2b     0.666667 0.333333 0.381
Ti     3    2b     0.666667 0.333333 0.876
Cl     1    6c     0.8449 0.0176 0.2736
Cl     2    6c     0.3157 0.4926 0.122
Cl     3    6c     0.6520 0.1606 0.123
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [    2/5]
```

Transformed high symmetry structure in the subgroup basis

```
173
12.135008 12.135008 6.055000 90.000000 90.000000 120.000000
7
Ti       1        2a       0.000000         0.000000         0.600000
Ti       1_2      2b       0.666667         0.333333         0.600000
Ti       1_3      2b       0.333333         0.666667         0.600000
K        1        6c       0.333334         0.000000         0.350000
Cl       1        6c       0.160000         0.000000         0.850000
Cl       1_2      6c       0.826667         0.333333         0.850000
Cl       1_3      6c       0.493333         0.666667         0.850000
```

Atom pairings and distances

Atom Mappings

WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,3/5)	Ti1	(0,0,0.52800)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,3/5)	Ti2	(2/3,1/3,0.38100)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,3/5)	Ti3	(1/3,2/3,0.37600)
6c	(x,y,z)	K1	(1/3,0,0.35000)	K1	(0.33700,0.99600,0.18000)
6c	(x,y,z)	Cl1	(0.16000,0,0.85000)	Cl1	(0.15510,0.98240,0.77360)
6c	(x,y,z)	Cl1_2	(0.82667,1/3,0.85000)	Cl2	(0.82310,0.31570,0.62200)
6c	(x,y,z)	Cl1_3	(0.49333,2/3,0.85000)	Cl3	(0.49140,0.65200,0.62300)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	-0.0720	0.4360
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	-0.2190	1.3260
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	-0.2240	1.3563
6c	(x,y,z)	K1	0.0037	-0.0040	-0.1700	1.0325
6c	(x,y,z)	Cl1	-0.0049	-0.0176	-0.0764	0.5005
6c	(x,y,z)	Cl1_2	-0.0036	-0.0176	-0.2280	1.3944
6c	(x,y,z)	Cl1_3	-0.0019	-0.0147	-0.2270	1.3847

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 1.3944 Å
Total distortion amplitude: 6.2166 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.17461)

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,3/5)	Ti1	(0,0,0.70261)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,3/5)	Ti2	(2/3,1/3,0.55561)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,3/5)	Ti3	(1/3,2/3,0.55061)
6c	(x,y,z)	K1	(1/3,0,0.35000)	K1	(0.33700,0.99600,0.35461)
6c	(x,y,z)	Cl1	(0.16000,0,0.85000)	Cl1	(0.15510,0.98240,0.94821)

6c	(x,y,z)	Cl1_2	(0.82667,1/3,0.85000)	Cl2	(0.82310,0.31570,0.79661)
6c	(x,y,z)	Cl1_3	(0.49333,2/3,0.85000)	Cl3	(0.49140,0.65200,0.79761)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	0.1026	0.6213
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	-0.0444	0.2688
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	-0.0494	0.2990
6c	(x,y,z)	K1	0.0037	-0.0040	0.0046	0.0853
6c	(x,y,z)	Cl1	-0.0049	-0.0176	0.0982	0.6246
6c	(x,y,z)	Cl1_2	-0.0036	-0.0176	-0.0534	0.3780
6c	(x,y,z)	Cl1_3	-0.0019	-0.0147	-0.0524	0.3587

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.6246 Å
Total distortion amplitude: 2.2603 Å

Symmetry Modes Summary

Atoms	WP	Modes
Cl1	6*h*	GM1+(1) GM2+(1) GM2-(1) K1(2) K2(1) K3(1) K4(2)
K1	2*d*	GM2-(1) K1(1) K4(1)
Ti1	2*a*	GM2-(1) K3(1) K4(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.2497
(0,0,0)	GM2+	(a)	P6_3/m (176)	1	0.7416
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.1038
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.1802
(1/3,1/3,0)	K2	(a,0)	P6_322 (182)	1	0.0105
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	2.1073

(1/3,1/3,0)	K4	(a,0)	P6_3/m (176)	4	0.1116

Global distortion: 2.2603 Å

Normalized Symmetry modes

The modes are normalized to the low symmetry unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.019423	0.000000	-0.000000
Cl1_2	0.019423	0.000000	-0.000000
Cl1_3	0.019423	0.000000	-0.000000

Irrep GM2+

GM2+ Mode Cl1 1

Atom	δx	δy	δz
Cl1	-0.011214	-0.022428	0.000000
Cl1_2	-0.011214	-0.022428	0.000000
Cl1_3	-0.011214	-0.022428	0.000000

Irrep GM2-

GM2- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.067423
Ti1_2	0.000000	0.000000	0.067423
Ti1_3	0.000000	0.000000	0.067423

GM2- Mode K1 1

Atom	δx	δy	δz
K1	0.000000	0.000000	0.067423

GM2- Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.038927
Cl1_2	0.000000	0.000000	0.038927
Cl1_3	0.000000	0.000000	0.038927

Irrep K1

K1 Mode K1 1

Atom	δx	δy	δz
K1	0.033642	0.000000	-0.000000

K1 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.000000
Cl1_2	-0.013734	-0.027469	0.000000
Cl1_3	0.013734	0.027469	-0.000000

K1 Mode Cl1 2

Atom	δx	δy	δz
Cl1	0.027469	0.000000	-0.000000
Cl1_2	-0.013734	0.000000	0.000000
Cl1_3	-0.013734	0.000000	0.000000

Irrep K2

K2 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.000000
Cl1_2	0.000000	0.000000	0.047675
Cl1_3	0.000000	0.000000	-0.047675

Irrep K3

K3 Mode Ti1 1

Atom	δx	δy	δz

Ti1	0.000000	0.000000	0.095351
Ti1_2	0.000000	0.000000	-0.047675
Ti1_3	0.000000	0.000000	-0.047675

K3 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.055051
Cl1_2	0.000000	0.000000	-0.027525
Cl1_3	0.000000	0.000000	-0.027525

Irrep K4

K4 Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.000000
Ti1_2	0.000000	0.000000	0.082576
Ti1_3	0.000000	0.000000	-0.082576

K4 Mode K1 1

Atom	δx	δy	δz
K1	-0.019423	-0.038847	0.000000

K4 Mode Cl1 1

Atom	δx	δy	δz
Cl1	0.000000	0.000000	0.000000
Cl1_2	0.023789	0.000000	-0.000000
Cl1_3	-0.023789	-0.000000	0.000000

K4 Mode Cl1 2

Atom	δx	δy	δz
Cl1	-0.015859	-0.031718	0.000000
Cl1_2	0.007930	0.015859	-0.000000
Cl1_3	0.007930	0.015859	-0.000000

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[       1       0       0  ] [        0]
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM1+} = 0.2497 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Cl1 1
0.2497

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	0.0000	0.0000	0.0000
Cl1	0.0194	0.0000	-0.0000
Cl1_2	0.0194	0.0000	-0.0000
Cl1_3	0.0194	0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2+

Direction: (a)

Isotropy Subgroup: 176 P6_3/m C6h-2

Transformation matrix:

```
[       1       0       0  ] [        0]
```

```
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM2+} = 0.7416 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Cl1 1
0.7416

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	0.0000	0.0000	0.0000
Cl1	-0.0112	-0.0224	0.0000
Cl1_2	-0.0112	-0.0224	0.0000
Cl1_3	-0.0112	-0.0224	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[       1       0       0  ] [        0]
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM2-} = 0.1038 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	K1 1	Cl1 1
0.4208	0.6589	-0.6235

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0284
Ti1_2	0.0000	0.0000	0.0284
Ti1_3	0.0000	0.0000	0.0284
K1	0.0000	0.0000	0.0444
Cl1	0.0000	0.0000	-0.0243
Cl1_2	0.0000	0.0000	-0.0243
Cl1_3	0.0000	0.0000	-0.0243

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0  ] [       0]
[      1      1      0  ] [       0]
[      0      0      1  ] [       0]
```

The amplitude of this distortion is:
A_{K1}= 0.1802 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

K1 1	Cl1 1	Cl1 2
0.9346	0.2996	-0.1919

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	0.0314	0.0000	-0.0000
Cl1	-0.0053	-0.0000	0.0000
Cl1_2	-0.0015	-0.0082	0.0000
Cl1_3	0.0067	0.0082	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K2

Direction: (a,0)

Isotropy Subgroup: 182 P6_322 D6-6

Transformation matrix:

```
[      2     -1      0  ] [       0]
[      1      1      0  ] [       0]
[      0      0      1  ] [     1/4]
```

The amplitude of this distortion is:
A_{K2}= 0.0105 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Cl1 1
-0.0105

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000

K1	0.0000	0.0000	0.0000
Cl1	0.0000	0.0000	0.0000
Cl1_2	0.0000	0.0000	-0.0477
Cl1_3	0.0000	0.0000	0.0477

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K3}= 2.1073 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	Cl1 1
0.4960	0.8683

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0473
Ti1_2	0.0000	0.0000	-0.0236
Ti1_3	0.0000	0.0000	-0.0236
K1	0.0000	0.0000	0.0000
Cl1	0.0000	0.0000	0.0478
Cl1_2	0.0000	0.0000	-0.0239
Cl1_3	0.0000	0.0000	-0.0239

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K4

Direction: (a,0)

Isotropy Subgroup: 176 P6_3/m C6h-2

Transformation matrix:

```
[      2     -1      0 ] [       0]
[      1      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{K4}= 0.1116 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	K1 1	Cl1 1	Cl1 2
0.2712	0.9225	-0.0284	0.2730

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0224
Ti1_3	0.0000	0.0000	-0.0224
K1	-0.0179	-0.0358	0.0000
Cl1	-0.0043	-0.0087	0.0000
Cl1_2	0.0015	0.0043	-0.0000
Cl1_3	0.0028	0.0043	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

http://www.cryst.ehu.es cryst@wm.lc.ehu.es

KTiBr3

ef: Liesbet Jongen, Thomas Gloger, Jan Beekhuizen, and Gerd Meyer Z. Anorg. Allg. Chem. 2005, 631, 582_586.

Symmetry mode analysis

High symmetry structure

```
194
7.37565 7.37565 6.344 90 90 120
3
Ti     1    2a     0.0 0.0 0.0
K      1    2d     0.333333 0.666667 0.75
Br     1    6h     0.16 0.32 0.25
```

Low symmetry structure

```
173
12.775 12.775 6.344 90.00 90.00 120.00
7
K      1    6c     0.3606 0.9996 0.523
Ti     1    2a     0.0 0.0 0.504
Ti     2    2b     0.333333 0.6666667 0.266
Ti     3    2b     0.333333 0.666667 0.767
Br     1    6c     0.1894 0.0949 0.7712
Br     2    6c     0.3285 0.8315 0.015
Br     3    6c     0.5031 0.8319 0.531
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [     2/5]
```

Transformed high symmetry structure in the subgroup basis

```
173
12.775001 12.775001 6.344000 90.000000 90.000000 120.000000
7
Ti       1        2a       0.000000         0.000000         0.600000
Ti       1_2      2b       0.666667         0.333333         0.600000
Ti       1_3      2b       0.333333         0.666667         0.600000
K        1        6c       0.333334         0.000000         0.350000
Br       1        6c       0.160000         0.000000         0.850000
Br       1_2      6c       0.826667         0.333333         0.850000
Br       1_3      6c       0.493333         0.666667         0.850000
```

Atom pairings and distances

Atom Mappings

WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,3/5)	Ti1	(0,0,0.50400)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,3/5)	Ti2	(2/3,1/3,0.76600)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,3/5)	Ti3	(1/3,2/3,0.76700)
6c	(x,y,z)	K1	(1/3,0,0.35000)	K1	(0.36060,0.99960,0.52300)
6c	(x,y,z)	Br1	(0.16000,0,0.85000)	Br1	(0.18940,0.09490,0.77120)
6c	(x,y,z)	Br1_2	(0.82667,1/3,0.85000)	Br3	(0.83190,0.32880,0.03100)
6c	(x,y,z)	Br1_3	(0.49333,2/3,0.85000)	Br2	(0.50300,0.67150,0.01500)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	-0.0960	0.6090
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	0.1660	1.0531
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	0.1670	1.0594
6c	(x,y,z)	K1	0.0273	-0.0004	0.1730	1.1522
6c	(x,y,z)	Br1	0.0294	0.0949	-0.0788	1.1855
6c	(x,y,z)	Br1_2	0.0052	-0.0045	0.1810	1.1533
6c	(x,y,z)	Br1_3	0.0097	0.0048	0.1650	1.0522

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 1.1855 Å
Total distortion amplitude: 6.0188 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.10384)

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,3/5)	Ti1	(0,0,0.40016)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,3/5)	Ti2	(2/3,1/3,0.66216)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,3/5)	Ti3	(1/3,2/3,0.66316)
6c	(x,y,z)	K1	(1/3,0,0.35000)	K1	(0.36060,0.99960,0.41916)
6c	(x,y,z)	Br1	(0.16000,0,0.85000)	Br1	(0.18940,0.09490,0.66736)

6c	(x,y,z)	Br1_2	(0.82667,1/3,0.85000)	Br3	(0.83190,0.32880,0.92716)
6c	(x,y,z)	Br1_3	(0.49333,2/3,0.85000)	Br2	(0.50300,0.67150,0.91116)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	-0.1998	1.2678
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	0.0622	0.3943
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	0.0632	0.4007
6c	(x,y,z)	K1	0.0273	-0.0004	0.0692	0.5618
6c	(x,y,z)	Br1	0.0294	0.0949	-0.1826	1.5805
6c	(x,y,z)	Br1_2	0.0052	-0.0045	0.0772	0.5013
6c	(x,y,z)	Br1_3	0.0097	0.0048	0.0612	0.4025

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 1.5805 Å
Total distortion amplitude: 4.8175 Å

Symmetry Modes Summary

Atoms	WP	Modes
Br1	6*h*	GM1+(1) GM2+(1) GM2-(1) K1(2) K2(1) K3(1) K4(2)
K1	2*d*	GM2-(1) K1(1) K4(1)
Ti1	2*a*	GM2-(1) K3(1) K4(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.0596
(0,0,0)	GM2+	(a)	P6_3/m (176)	1	1.4895
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	1.2092
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	1.0922
(1/3,1/3,0)	K2	(a,0)	P6_322 (182)	1	0.1758
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	3.7289

(1/3,1/3,0)	K4	(a,0)	P6_3/m (176)	4	2.0966

Global distortion: 4.8175 Å

Detailed information

KTiI3

ref: Liesbet Jongen, Thomas Gloger, Jan Beekhuizen, and Gerd Meyer Z. Anorg. Allg. Chem. 2005, 631, 582_586

Symmetry mode analysis

High symmetry structure

```
194
7.815 7.815 6.6462 90 90 120
3
Ti     1    2a     0.0 0.0 0.0
K      1    2d     0.333333 0.666667 0.75
I      1    6h     0.16 0.32 0.25
```

Low symmetry structure

```
173
13.536 13.536 6.6462 90.00 90.00 120.00
7
K      1    6c     0.0059 0.321 0.907
Ti     1    2a     0.0 0.0 0.604
Ti     2    2b     0.666667 0.333333 0.772
Ti     3    2b     0.666667 0.333333 0.273
I      1    6c     0.1587 0.1788 0.8520
I      2    6c     0.4813 0.2827 0.0168
I      3    6c     0.8568 0.3858 0.5152
```

Transformation matrix

```
[      1     -2      0 ] [       0]
[      2     -1      0 ] [       0]
[      0      0      1 ] [   -1/5]
```

Transformed high symmetry structure in the subgroup basis

```
173
13.535977 13.535977 6.646200 90.000000 90.000000 120.000000
7
Ti       1        2a       0.000000         0.000000         0.200000
Ti       1_2      2b       0.666667         0.333333         0.200000
Ti       1_3      2b       0.333333         0.666667         0.200000
K        1        6c       0.333334         0.000000         0.950000
I        1        6c       0.160000         0.000000         0.450000
I        1_2      6c       0.826667         0.333333         0.450000
I        1_3      6c       0.493333         0.666667         0.450000
```

Atom pairings and distances

Atom Mappings

WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,1/5)	Ti1	(0,0,0.10400)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,1/5)	Ti3	(2/3,1/3,3/11)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,1/5)	Ti2	(1/3,2/3,3/11)
6c	(x,y,z)	K1	(1/3,0,0.95000)	K1	(0.31510,0.99410,0.90700)
6c	(x,y,z)	I1	(0.16000,0,0.45000)	I1	(0.17880,0.02010,0.35200)
6c	(x,y,z)	I1_2	(0.82667,1/3,0.45000)	I3	(0.85680,0.38580,0.51520)
6c	(x,y,z)	I1_3	(0.49333,2/3,0.45000)	I2	(0.51870,0.71730,0.51680)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	-0.0960	0.6380
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	0.0730	0.4852
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	0.0720	0.4785
6c	(x,y,z)	K1	-0.0182	-0.0059	-0.0430	0.3595
6c	(x,y,z)	I1	0.0188	0.0201	-0.0980	0.7027
6c	(x,y,z)	I1_2	0.0301	0.0525	0.0652	0.7542
6c	(x,y,z)	I1_3	0.0254	0.0506	0.0668	0.7412

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.7542 Å
Total distortion amplitude: 3.4914 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.00147)

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ti1	(0,0,1/5)	Ti1	(0,0,0.10253)
2b	(1/3,2/3,z)	Ti1_2	(2/3,1/3,1/5)	Ti3	(2/3,1/3,0.27153)
2b	(1/3,2/3,z)	Ti1_3	(1/3,2/3,1/5)	Ti2	(1/3,2/3,0.27053)
6c	(x,y,z)	K1	(1/3,0,0.95000)	K1	(0.31510,0.99410,0.90553)
6c	(x,y,z)	I1	(0.16000,0,0.45000)	I1	(0.17880,0.02010,0.35053)

6c	(x,y,z)	I1_2	(0.82667,1/3,0.45000)	I3	(0.85680,0.38580,0.51373)
6c	(x,y,z)	I1_3	(0.49333,2/3,0.45000)	I2	(0.51870,0.71730,0.51533)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ti1	0.0000	0.0000	-0.0975	0.6478
2b	(1/3,2/3,z)	Ti1_2	0.0000	0.0000	0.0715	0.4754
2b	(1/3,2/3,z)	Ti1_3	0.0000	0.0000	0.0705	0.4688
6c	(x,y,z)	K1	-0.0182	-0.0059	-0.0445	0.3673
6c	(x,y,z)	I1	0.0188	0.0201	-0.0995	0.7117
6c	(x,y,z)	I1_2	0.0301	0.0525	0.0637	0.7487
6c	(x,y,z)	I1_3	0.0254	0.0506	0.0653	0.7354

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.7487 Å
Total distortion amplitude: 3.4911 Å

Symmetry Modes Summary

Atoms	WP	Modes
I1	6*h*	GM1+(1) GM2+(1) GM2-(1) K1(2) K2(1) K3(1) K4(2)
K1	2*d*	GM2-(1) K1(1) K4(1)
Ti1	2*a*	GM2-(1) K3(1) K4(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P6_3/mmc (194)	1	0.2431
(0,0,0)	GM2+	(a)	P6_3/m (176)	1	2.0424
(0,0,0)	GM2-	(a)	P6_3mc (186)	3	0.8124
(1/3,1/3,0)	K1	(a,0)	P6_3/mcm (193)	3	0.5402
(1/3,1/3,0)	K2	(a,0)	P6_322 (182)	1	0.0184
(1/3,1/3,0)	K3	(a,0)	P6_3cm (185)	2	2.5346

(1/3,1/3,0)	K4	(a,0)	P6_3/m (176)	4	0.7619

Global distortion: 3.4911 Å

Normalized Symmetry modes

The modes are normalized to the low symmetry unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode I1 1

Atom	δx	δy	δz
I1	0.017413	0.000000	-0.000000
I1_2	0.017413	0.000000	-0.000000
I1_3	0.017413	0.000000	-0.000000

Irrep GM2+

GM2+ Mode I1 1

Atom	δx	δy	δz
I1	-0.010053	-0.020107	0.000000
I1_2	-0.010053	-0.020107	0.000000
I1_3	-0.010053	-0.020107	0.000000

Irrep GM2-

GM2- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.061426
Ti1_2	0.000000	0.000000	0.061426
Ti1_3	0.000000	0.000000	0.061426

GM2- Mode K1 1

Atom	δx	δy	δz
K1	0.000000	0.000000	0.061426

GM2- Mode I1 1

Atom	δx	δy	δz
I1	0.000000	0.000000	0.035464
I1_2	0.000000	0.000000	0.035464
I1_3	0.000000	0.000000	0.035464

Irrep K1

K1 Mode K1 1

Atom	δx	δy	δz
K1	0.030160	0.000000	-0.000000

K1 Mode I1 1

Atom	δx	δy	δz
I1	0.000000	0.000000	0.000000
I1_2	-0.012313	-0.024626	0.000000
I1_3	0.012313	0.024626	-0.000000

K1 Mode I1 2

Atom	δx	δy	δz
I1	0.024626	0.000000	-0.000000
I1_2	-0.012313	-0.000000	0.000000
I1_3	-0.012313	-0.000000	0.000000

Irrep K2

K2 Mode I1 1

Atom	δx	δy	δz
I1	0.000000	0.000000	0.000000
I1_2	0.000000	0.000000	0.043435
I1_3	0.000000	0.000000	-0.043435

Irrep K3

K3 Mode Ti1 1

Atom	δx	δy	δz

Ti1	0.000000	0.000000	0.086869
Ti1_2	0.000000	0.000000	-0.043435
Ti1_3	0.000000	0.000000	-0.043435

K3 Mode I1 1

Atom	δx	δy	δz
I1	0.000000	0.000000	0.050154
I1_2	0.000000	0.000000	-0.025077
I1_3	0.000000	0.000000	-0.025077

Irrep K4

K4 Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.000000
Ti1_2	0.000000	0.000000	0.075231
Ti1_3	0.000000	0.000000	-0.075231

K4 Mode K1 1

Atom	δx	δy	δz
K1	-0.017413	-0.034826	0.000000

K4 Mode I1 1

Atom	δx	δy	δz
I1	0.000000	0.000000	0.000000
I1_2	0.021327	0.000000	-0.000000
I1_3	-0.021327	-0.000000	0.000000

K4 Mode I1 2

Atom	δx	δy	δz
I1	-0.014218	-0.028435	0.000000
I1_2	0.007109	0.014218	-0.000000
I1_3	0.007109	0.014218	-0.000000

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 194 P6_3/mmc D6h-4

Transformation matrix:

```
[       1       0       0  ] [        0]
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM1+} = 0.2431 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

I1 1
0.2431

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	0.0000	0.0000	0.0000
I1	0.0174	0.0000	-0.0000
I1_2	0.0174	0.0000	-0.0000
I1_3	0.0174	0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2+

Direction: (a)

Isotropy Subgroup: 176 P6_3/m C6h-2

Transformation matrix:

```
[       1       0       0  ] [        0]
```

```
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM2+}= 2.0424 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

I1 1
-2.0424

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	0.0000	0.0000	0.0000
I1	0.0101	0.0201	-0.0000
I1_2	0.0101	0.0201	-0.0000
I1_3	0.0101	0.0201	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2-

Direction: (a)

Isotropy Subgroup: 186 P6_3mc C6v-4

Transformation matrix:

```
[       1       0       0  ] [        0]
[       0       1       0  ] [        0]
[       0       0       1  ] [        0]
```

The amplitude of this distortion is:
A_{GM2-}= 0.8124 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	K1 1	I1 1
0.2979	-0.8911	0.3424

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0183
Ti1_2	0.0000	0.0000	0.0183
Ti1_3	0.0000	0.0000	0.0183
K1	0.0000	0.0000	-0.0547
I1	0.0000	0.0000	0.0121
I1_2	0.0000	0.0000	0.0121
I1_3	0.0000	0.0000	0.0121

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: K = (1/3,1/3,0)

Irrep: K1

Direction: (a,0)

Isotropy Subgroup: 193 P6_3/mcm D6h-3

Transformation matrix:

```
[      2     -1      0 ] [       0]
[      1      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{K1}= 0.5402 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

K1 1	I1 1	I1 2
-0.9381	-0.0689	0.3395

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000
K1	-0.0283	-0.0000	0.0000
I1	0.0084	0.0000	-0.0000
I1_2	-0.0033	0.0017	0.0000
I1_3	-0.0050	-0.0017	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K2

Direction: (a,0)

Isotropy Subgroup: 182 P6_322 D6-6

Transformation matrix:

```
[      2     -1      0  ] [       0]
[      1      1      0  ] [       0]
[      0      0      1  ] [     1/4]
```

The amplitude of this distortion is:
A_{K2}= 0.0184 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

I1 1
-0.0184

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0000
Ti1_3	0.0000	0.0000	0.0000

K1	0.0000	0.0000	0.0000
I1	0.0000	0.0000	0.0000
I1_2	0.0000	0.0000	-0.0434
I1_3	0.0000	0.0000	0.0434

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K3

Direction: (a,0)

Isotropy Subgroup: 185 P6_3cm C6v-3

Transformation matrix:

```
[      2     -1      0 ] [      0]
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{K3}= 2.5346 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	I1 1
-0.5102	-0.8601

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	-0.0443
Ti1_2	0.0000	0.0000	0.0222
Ti1_3	0.0000	0.0000	0.0222
K1	0.0000	0.0000	0.0000
I1	0.0000	0.0000	-0.0431
I1_2	0.0000	0.0000	0.0216
I1_3	0.0000	0.0000	0.0216

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: K4

Direction: (a,0)

Isotropy Subgroup: 176 P6_3/m C6h-2

Transformation matrix:

```
[      2     -1      0 ] [       0]
[      1      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{K4}= 0.7619 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ti1 1	K1 1	I1 1	I1 2
0.0087	0.2223	0.1184	0.9677

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ti1	0.0000	0.0000	0.0000
Ti1_2	0.0000	0.0000	0.0007
Ti1_3	0.0000	0.0000	-0.0007
K1	-0.0039	-0.0077	0.0000
I1	-0.0138	-0.0275	0.0000
I1_2	0.0094	0.0138	-0.0000
I1_3	0.0044	0.0138	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

http://www.cryst.ehu.es cryst@wm.lc.ehu.es

SrZrO3-Pnma-20C

Ref: Howard CJ, Knight KS, Kennedy BJ, et al.JOURNAL OF PHYSICS-CONDENSED MATTER (2000) 12 L677-L683;Kennedy BJ, Howard CJ, Chakoumakos BC, PHYSICAL REVIEW B (1999) 59, 4023-4027 Pu

Symmetry mode analysis

High symmetry structure

```
221
4.1514 4.1514 4.1514 90 90 90
3
Zr      1       1a      0.000000        0.000000        0.000000
Sr      2       1b      0.500000        0.500000        0.500000
O       3       3d      0.500000        0.000000        0.000000
```

Low symmetry structure

```
62
5.81981 8.20664 5.7963 90 90 90
4
Zr      1       4a      0.000000        0.000000        0.000000
Sr      2       4c      0.024500        0.250000        0.494100
O       3       4c      0.984900        0.250000        0.928500
O       4       8d      0.284100        0.035620        0.216500
```

Transformation matrix

```
[     1     0    -1 ] [      0]
[     0     2     0 ] [      0]
[     1     0     1 ] [      0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
062
5.870966 8.302800 5.870966 90.000000 90.000000 90.000000
4
Zr      1       4a      0.000000        0.000000        0.000000
Sr      2       4c      0.500000        0.250000        0.000000
O       3       8d      0.250000        0.000000        0.750000
O       3_2     4c      0.500000        0.750000        0.500000
```

Atom pairings and distances

Atom Mappings				
WP	**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**

4a	(0,0,0)	Zr1	(0.000000,0.000000,0.000000)	Zr1	(0.000000,0.000000,0.000000)
4c	(x,1/4,z)	Sr2	(0.500000,0.250000,0.000000)	Sr2	(0.524500,0.250000,0.005900)
8d	(x,y,z)	O3	(0.250000,0.000000,0.750000)	O4	(0.215900,0.964380,0.716500)
4c	(x,1/4,z)	O3_2	(0.500000,0.750000,0.500000)	O3	(0.515100,0.750000,0.428500)

WP		**Atom**	**Atomic Displacements**			
			$\mathbf{u_x}$	$\mathbf{u_y}$	$\mathbf{u_z}$	**|u|**
4a	(0,0,0)	Zr1	0.0000	0.0000	0.0000	0.0000
4c	(x,1/4,z)	Sr2	0.0245	0.0000	0.0059	0.1480
8d	(x,y,z)	O3	-0.0341	-0.0356	-0.0335	0.4077
4c	(x,1/4,z)	O3_2	0.0151	0.0000	-0.0715	0.4290

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4290 Å
Total distortion amplitude: 1.4675 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3	3*d*	R4+(1) R5+(1) X5+(1) M2+(1) M3+(1)
Sr2	1*b*	R5+(1) X5+(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4+	(a,a,0)	Imma (74)	1	1.1851
(1/2,1/2,1/2)	R5+	(-a,a,0)	Imma (74)	2	0.0693
(0,1/2,0)	X5+	(0,a,0,0,0,0)	Cmcm (63)	2	0.3379
(1/2,1/2,0)	M2+	(0,0,a)	P4/mbm (127)	1	0.0070
(1/2,1/2,0)	M3+	(0,0,a)	P4/mbm (127)	1	0.7938

Global distortion: 1.4675 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep R4+

R4+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.030110	-0.000000
O3_2	0.000000	0.000000	0.060221

Irrep R5+

R5+ Mode Sr2 1

Atom	δx	δy	δz
Sr2	0.000000	0.000000	-0.085165

R5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.030110	0.000000
O3_2	0.000000	0.000000	0.060221

Irrep X5+

X5+ Mode Sr2 1

Atom	δx	δy	δz
Sr2	-0.085165	0.000000	0.000000

X5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	-0.085165	0.000000	0.000000

Irrep M2+

M2+ Mode O3 1

Atom	δx	δy	δz
O3	-0.042582	0.000000	0.042582

O3_2	0.000000	0.000000	0.000000

Irrep M3+

M3+ Mode O3 1

Atom	δx	δy	δz
O3	-0.042582	0.000000	-0.042582
O3_2	0.000000	0.000000	0.000000

K-vector: R = (1/2,1/2,1/2)

Irrep: R4+

Direction: (a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1      0     -1 ] [      0]
[      0      2      0 ] [      0]
[      1      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{R4+}= 1.1851 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-1.1851

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	0.0000	-0.0301	0.0000
O3_2	0.0000	0.0000	-0.0602

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: R5+

Direction: (-a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1      0      1  ] [       0]
[      0     -2      0  ] [       0]
[      1      0     -1  ] [       0]
```

The amplitude of this distortion is:
A_{R5+}= 0.0693 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Sr2 1	O3 1
-0.9995	-0.0311

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0851
O3	0.0000	0.0009	-0.0000
O3_2	0.0000	0.0000	-0.0019

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: X = (0,1/2,0)

Irrep: X5+

Direction: (0,a,0,0,0,0)

Isotropy Subgroup: 63 Cmcm D2h-17

Transformation matrix:

```
[      1       1       0  ] [       0]
[      0       0      -2  ] [       0]
[     -1       1       0  ] [       0]
```

The amplitude of this distortion is:
A_{X5+} = 0.3379 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Sr2 1	O3 1
-0.8513	-0.5247

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0725	-0.0000	-0.0000
O3	0.0000	0.0000	0.0000
O3_2	0.0447	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: M = (1/2,1/2,0)

Irrep: M2+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1       1       0  ] [     1/2]
[      0       0       1  ] [       0]
[      1      -1       0  ] [     1/2]
```

The amplitude of this distortion is:
A_{M2+} = 0.0070 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1

0.0070

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	-0.0426	0.0000	0.0426
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: M3+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1      1      0 ] [      0]
[      0      0      1 ] [      0]
[      1     -1      0 ] [      0]
```

The amplitude of this distortion is:
A_{M3+} = 0.7938 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
0.7938

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Zr1	0.0000	0.0000	0.0000
Sr2	0.0000	0.0000	0.0000
O3	-0.0426	0.0000	-0.0426
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

NaTaO3-Cmcm

Ref:Kennedy, B.J.;Prodjosantoso, A.K.;Howard, C.J., Journal of Physics: Condensed Matter (1999) 11, 6319-6327

Symmetry mode analysis

High symmetry structure

```
221
3.9313 3.9313 3.9313 90 90 90
3
Ta       1        1a       0.000000        0.000000        0.000000
Na       2        1b       0.500000        0.500000        0.500000
O        3        3d       0.500000        0.000000        0.000000
```

Low symmetry structure

```
63
7.83729 7.84887 7.85728 90 90 90
6
Ta       1        8d       0.250000        0.250000        0.000000
Na       1        4c       0.000000        0.008000        0.250000
Na       2        4c       0.000000        0.507000        0.250000
O        1        8e       0.225300        0.000000        0.000000
O        2        8f       0.000000        0.273900        0.020000
O        3        8g       0.273700        0.247800        0.250000
```

Transformation matrix

```
[    -2     0     0 ] [    1/2]
[     0    -2     0 ] [    1/2]
[     0     0     2 ] [      0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
063
7.862600 7.862600 7.862600 90.000000 90.000000 90.000000
6
Ta       1        8d       0.250000        0.250000        0.000000
Na       2        4c       0.000000        0.000000        0.250000
Na       2_2      4c       0.500000        0.000000        0.750000
O        3        8f       0.000000        0.250000        0.000000
O        3_2      8e       0.250000        0.000000        0.000000
O        3_3      8g       0.250000        0.250000        0.250000
```

Atom pairings and distances

Atom Mappings

WP		Atom	Reference Struc.	Atom	Low Sym Struc.
8d	(1/4,1/4,0)	Ta1	(0.250000,0.250000,0.000000)	Ta1	(0.250000,0.250000,0.000000)
4c	(0,y,1/4)	Na2	(0.000000,0.000000,0.250000)	Na1	(0.000000,0.008000,0.250000)
4c	(0,y,1/4)	Na2_2	(0.500000,0.000000,0.750000)	Na2	(0.500000,0.993000,0.750000)
8f	(0,y,z)	O3	(0.000000,0.250000,0.000000)	O2	(0.000000,0.273900,0.020000)
8e	(x,0,0)	O3_2	(0.250000,0.000000,0.000000)	O1	(0.225300,0.000000,0.000000)
8g	(x,y,1/4)	O3_3	(0.250000,0.250000,0.250000)	O3	(0.273700,0.247800,0.250000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
8d	(1/4,1/4,0)	Ta1	0.0000	0.0000	0.0000	0.0000
4c	(0,y,1/4)	Na2	0.0000	0.0080	0.0000	0.0629
4c	(0,y,1/4)	Na2_2	0.0000	-0.0070	0.0000	0.0550
8f	(0,y,z)	O3	0.0000	0.0239	0.0200	0.2450
8e	(x,0,0)	O3_2	-0.0247	0.0000	0.0000	0.1942
8g	(x,y,1/4)	O3_3	0.0237	-0.0022	0.0000	0.1871

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2450 Å
Total distortion amplitude: 0.7382 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3	3*d*	R4+(1) R5+(1) X5+(1) M3+(1) M4+(1)
Na2	1*b*	R5+(1) X5+(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4+	(0,0,a)	I4/mcm (140)	1	0.4859
(1/2,1/2,1/2)	R5+	(0,0,a)	I4/mmm (139)	2	0.0419
(0,1/2,0)	X5+	(0,0,-a,a,0,0)	Pmma (51)	2	0.1229

(1/2,1/2,0)	M3+	(a,0,0)	P4/mbm (127)	1	0.5404
(1/2,1/2,0)	M4+	(a,0,0)	P4/mmm (123)	1	0.0089

Global distortion: 0.7383 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep R4+

R4+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	-0.044966
O3_2	0.000000	0.000000	0.000000
O3_3	-0.044966	0.000000	0.000000

Irrep R5+

R5+ Mode Na2 1

Atom	δx	δy	δz
Na2	0.000000	-0.063592	0.000000
Na2_2	0.000000	-0.063592	0.000000

R5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.044966
O3_2	0.000000	0.000000	0.000000
O3_3	-0.044966	0.000000	0.000000

Irrep X5+

X5+ Mode Na2 1

Atom	δx	δy	δz
Na2	0.000000	0.063592	-0.000000
Na2_2	0.000000	-0.063592	0.000000

X5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	0.000000	0.000000
O3_3	0.000000	-0.063592	0.000000

Irrep M3+

M3+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.044966	0.000000
O3_2	0.044966	-0.000000	-0.000000
O3_3	0.000000	0.000000	0.000000

Irrep M4+

M4+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.044966	0.000000
O3_2	-0.044966	0.000000	0.000000
O3_3	0.000000	0.000000	0.000000

K-vector: R = (1/2,1/2,1/2)

Irrep: R4+

Direction: (0,0,a)

Isotropy Subgroup: 140 I4/mcm D4h-18

Transformation matrix:

```
[      1       1       0 ] [       0]
[      0       0       2 ] [       0]
[      1      -1       0 ] [       0]
```

The amplitude of this distortion is:
A_{R4+}= 0.4859 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-0.4859

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
Na2_2	0.0000	0.0000	0.0000
O3	0.0000	0.0000	0.0450
O3_2	0.0000	0.0000	0.0000
O3_3	0.0450	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: R5+

Direction: (0,0,a)

Isotropy Subgroup: 139 I4/mmm D4h-17

Transformation matrix:

```
[      1      1      0 ] [     1/2]
[      0      0      2 ] [       0]
[      1     -1      0 ] [     1/2]
```

The amplitude of this distortion is:
A_{R5+} = 0.0419 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Na2 1	O3 1
-0.1877	-0.9822

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0119	-0.0000
Na2_2	0.0000	0.0119	-0.0000
O3	0.0000	0.0000	-0.0442
O3_2	0.0000	0.0000	0.0000
O3_3	0.0442	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: X = (0,1/2,0)

Irrep: X5+

Direction: (0,0,-a,a,0,0)

Isotropy Subgroup: 51 Pmma D2h-5

Transformation matrix:

```
[      0       1       0  ] [        0]
[      0       0      -1  ] [        0]
[     -2       0       0  ] [        0]
```

The amplitude of this distortion is:
A_{X5+}= 0.1229 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Na2 1	O3 1
0.9596	0.2815

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0610	-0.0000
Na2_2	0.0000	-0.0610	0.0000

O3	0.0000	0.0000	0.0000
O3_2	0.0000	0.0000	0.0000
O3_3	0.0000	-0.0179	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: M = (1/2,1/2,0)

Irrep: M3+

Direction: (a,0,0)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1     -1      0 ] [       0]
[      1      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{M3+}= 0.5404 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-0.5404

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
Na2_2	0.0000	0.0000	0.0000
O3	0.0000	0.0450	-0.0000
O3_2	-0.0450	0.0000	0.0000
O3_3	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: M4+

Direction: (a,0,0)

Isotropy Subgroup: 123 P4/mmm D4h-1

Transformation matrix:

```
[      1     -1      0 ] [     1/2]
[      1      1      0 ] [     1/2]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{M4+} = 0.0089 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
0.0089

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
Na2_2	0.0000	0.0000	0.0000
O3	0.0000	-0.0450	0.0000
O3_2	-0.0450	0.0000	0.0000
O3_3	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

NaTaO3-P4/mbm

Ref:Kennedy, B.J.;Prodjosantoso, A.K.;Howard, C.J., Journal of Physics: Condensed Matter (1999) 11, 6319-6327

Symmetry mode analysis

High symmetry structure

```
221
3.9313 3.9313 3.9313 90 90 90
3
Ta       1        1a       0.000000        0.000000        0.000000
Na       2        1b       0.500000        0.500000        0.500000
O        3        3d       0.500000        0.000000        0.000000
```

Low symmetry structure

```
127
3.9828 5.6745 5.6916 90 90 90
4
Na       1        2c       0.000000        0.500000        0.500000
Ta       1        2a       0.000000        0.000000        0.000000
O        1        2b       0.000000        0.000000        0.500000
O        2        4g       0.274100        0.774100        0.000000
```

Transformation matrix

```
[      1     -1      0 ] [       0]
[      1      1      0 ] [       0]
[      0      0      1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
127
5.559698 5.559698 3.931300 90.000000 90.000000 90.000000
4
Ta       1        2a       0.000000        0.000000        0.000000
Na       2        2c       0.500000        0.000000        0.500000
O        3        4g       0.250000        0.750000        0.000000
O        3_2      2b       0.500000        0.500000        0.500000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,0)	Ta1	(0.000000,0.000000,0.000000)	Ta1	(0.000000,0.000000,0.000000)

2c	(0,1/2,1/2)	Na2	(0.500000,0.000000,0.500000)	Na1	(0.500000,0.000000,0.500000)
4g	(x,x+1/2,0)	O3	(0.250000,0.750000,0.000000)	O2	(0.274100,0.774100,0.000000)
2b	(0,0,1/2)	O3_2	(0.500000,0.500000,0.500000)	O1	(0.500000,0.500000,0.500000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,0)	Ta1	0.0000	0.0000	0.0000	0.0000
2c	(0,1/2,1/2)	Na2	0.0000	0.0000	0.0000	0.0000
4g	(x,x+1/2,0)	O3	0.0241	0.0241	0.0000	0.1895
2b	(0,0,1/2)	O3_2	0.0000	0.0000	0.0000	0.0000

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1895 Å
Total distortion amplitude: 0.3790 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3	3*d*	**M3+(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,0)	M3+	(a,0,0)	P4/mbm (127)	1	0.3790

Global distortion: 0.3790 Å

Detailed information

NaTaO3

Ref:Kennedy, B.J.;Prodjosantoso, A.K.;Howard, C.J., Journal of Physics: Condensed Matter (1999) 11, 6319-6327

Symmetry mode analysis

High symmetry structure

```
221
3.9313 3.9313 3.9313 90 90 90
3
Ta       1        1a       0.000000         0.000000         0.000000
Na       2        1b       0.500000         0.500000         0.500000
O        3        3d       0.500000         0.000000         0.000000
```

Low symmetry structure

```
62
5.5212 7.7890 5.4768 90.00 90.00 90.00
4
Na       1        4c       0.518000         0.250000         0.002300
Ta       1        4a       0.000000         0.000000         0.000000
O        1        4c       -0.010100        0.250000         -0.061600
O        2        8d       0.284500         0.031000         0.214300
```

Transformation matrix

```
[      1      0     -1  ] [       0]
[      0      2      0  ] [       0]
[      1      0      1  ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
062
5.559698 7.862600 5.559698 90.000000 90.000000 90.000000
4
Ta       1        4a       0.000000         0.000000         0.000000
Na       2        4c       0.500000         0.250000         0.000000
O        3        8d       0.250000         0.000000         0.750000
O        3_2      4c       0.500000         0.750000         0.500000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4a	(0,0,0)	Ta1	(0.000000,0.000000,0.000000)	Ta1	(0.000000,0.000000,0.000000)

4c	(x,1/4,z)	Na2	(0.500000,0.250000,0.000000)	Na1	(0.518000,0.250000,0.002300)
8d	(x,y,z)	O3	(0.250000,0.000000,0.750000)	O2	(0.215500,0.969000,0.714300)
4c	(x,1/4,z)	O3_2	(0.500000,0.750000,0.500000)	O1	(0.510100,0.750000,0.438400)

WP		**Atom**	**Atomic Displacements**			
			$\mathbf{u_x}$	$\mathbf{u_y}$	$\mathbf{u_z}$	**|u|**
4a	(0,0,0)	Ta1	0.0000	0.0000	0.0000	0.0000
4c	(x,1/4,z)	Na2	0.0180	0.0000	0.0023	0.1009
8d	(x,y,z)	O3	-0.0345	-0.0310	-0.0357	0.3682
4c	(x,1/4,z)	O3_2	0.0101	0.0000	-0.0616	0.3471

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.3682 Å
Total distortion amplitude: 1.2678 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3	3*d*	R4+(1) R5+(1) X5+(1) M2+(1) M3+(1)
Na2	1*b*	R5+(1) X5+(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4+	(a,a,0)	Imma (74)	1	0.9718
(1/2,1/2,1/2)	R5+	(-a,a,0)	Imma (74)	2	0.0258
(0,1/2,0)	X5+	(0,a,0,0,0,0)	Cmcm (63)	2	0.2295
(1/2,1/2,0)	M2+	(0,0,a)	P4/mbm (127)	1	0.0133
(1/2,1/2,0)	M3+	(0,0,a)	P4/mbm (127)	1	0.7806

Global distortion: 1.2678 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative

displacements in this cell.

Irrep R4+

R4+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.031796	-0.000000
O3_2	0.000000	0.000000	0.063592

Irrep R5+

R5+ Mode Na2 1

Atom	δx	δy	δz
Na2	0.000000	0.000000	-0.089933

R5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.031796	0.000000
O3_2	0.000000	0.000000	0.063592

Irrep X5+

X5+ Mode Na2 1

Atom	δx	δy	δz
Na2	-0.089933	0.000000	0.000000

X5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	-0.089933	0.000000	0.000000

Irrep M2+

M2+ Mode O3 1

Atom	δx	δy	δz
O3	-0.044966	0.000000	0.044966
O3_2	0.000000	0.000000	0.000000

Irrep M3+

M3+ Mode O3 1

Atom	δx	δy	δz
O3	-0.044966	0.000000	-0.044966
O3_2	0.000000	0.000000	0.000000

K-vector: R = (1/2,1/2,1/2)

Irrep: R4+

Direction: (a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1      0     -1 ] [       0]
[      0      2      0 ] [       0]
[      1      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{R4+}= 0.9718 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-0.9718

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
O3	0.0000	-0.0318	0.0000
O3_2	0.0000	0.0000	-0.0636

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: R5+

Direction: (-a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1       0       1  ] [       0]
[      0      -2       0  ] [       0]
[      1       0      -1  ] [       0]
```

The amplitude of this distortion is:
A_{R5+} = 0.0258 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Na2 1	O3 1
-0.9925	0.1221

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0893
O3	0.0000	-0.0039	0.0000
O3_2	0.0000	0.0000	0.0078

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: X = (0,1/2,0)

Irrep: X5+

Direction: (0,a,0,0,0,0)

Isotropy Subgroup: 63 Cmcm D2h-17

Transformation matrix:

```
[      1       1       0  ] [       0]
[      0       0      -2  ] [       0]
```

```
[     -1      1      0 ] [       0]
```

The amplitude of this distortion is:
A_{X5+} = 0.2295 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Na2 1	O3 1
-0.8721	-0.4893

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0784	-0.0000	-0.0000
O3	0.0000	0.0000	0.0000
O3_2	0.0440	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: M = (1/2,1/2,0)

Irrep: M2+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1      1      0 ] [     1/2]
[      0      0      1 ] [       0]
[      1     -1      0 ] [     1/2]
```

The amplitude of this distortion is:
A_{M2+} = 0.0133 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-0.0133

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
O3	0.0450	-0.0000	-0.0450
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: M3+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1       1       0 ] [       0]
[      0       0       1 ] [       0]
[      1      -1       0 ] [       0]
```

The amplitude of this distortion is:
A_{M3+} = 0.7806 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
0.7806

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ta1	0.0000	0.0000	0.0000
Na2	0.0000	0.0000	0.0000
O3	-0.0450	0.0000	-0.0450
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

LaMnO3-Pnma-300K

Ref: . J. RodrÄ±guez-Carvajal, M. Hennion, F. Moussa, and A. H. Moudden L. Pinsard and A. Revcolevschi, Phys Rev B 57 (1998) R3189

Symmetry mode analysis

High symmetry structure

```
221
3.9475 3.9475 3.9475 90 90 90
3
Mn       1        1a       0.000000         0.000000         0.000000
La       2        1b       0.500000         0.500000         0.500000
O        3        3d       0.500000         0.000000         0.000000
```

Low symmetry structure

```
62
5.7473 7.6929 5.5367 90.00 90.00 90.00
4
Mn       1        4a       0.000000         0.000000         0.000000
La       2        4c       0.049000         0.250000         -0.507800
O        3        4c       0.487400         0.250000         -0.425500
O        4        8d       0.306600         0.038400         0.225600
```

Transformation matrix

```
[      1      0     -1  ] [       0]
[      0      2      0  ] [       0]
[      1      0      1  ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
062
5.582608 7.895000 5.582608 90.000000 90.000000 90.000000
4
Mn       1        4a       0.000000         0.000000         0.000000
La       2        4c       0.500000         0.250000         0.000000
O        3        8d       0.250000         0.000000         0.750000
O        3_2      4c       0.500000         0.750000         0.500000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4a	(0,0,0)	Mn1	(0.000000,0.000000,0.000000)	Mn1	(0.000000,0.000000,0.000000)

4c	(x,1/4,z)	La2	(0.500000,0.250000,0.000000)	La2	(0.549000,0.250000,0.007800)
8d	(x,y,z)	O3	(0.250000,0.000000,0.750000)	O4	(0.193400,0.961600,0.725600)
4c	(x,1/4,z)	O3_2	(0.500000,0.750000,0.500000)	O3	(0.512600,0.750000,0.425500)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4a	(0,0,0)	Mn1	0.0000	0.0000	0.0000	0.0000
4c	(x,1/4,z)	La2	0.0490	0.0000	0.0078	0.2770
8d	(x,y,z)	O3	-0.0566	-0.0384	-0.0244	0.4586
4c	(x,1/4,z)	O3_2	0.0126	0.0000	-0.0745	0.4218

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4586 Å
Total distortion amplitude: 1.6435 Å

Symmetry Modes Summary

Atoms	WP	Modes
O3	3*d*	R4+(1) R5+(1) X5+(1) M2+(1) M3+(1)
La2	1*b*	R5+(1) X5+(1)

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4+	(a,a,0)	Imma (74)	1	1.1945
(1/2,1/2,1/2)	R5+	(-a,a,0)	Imma (74)	2	0.0890
(0,1/2,0)	X5+	(0,a,0,0,0,0)	Cmcm (63)	2	0.5649
(1/2,1/2,0)	M2+	(0,0,a)	P4/mbm (127)	1	0.3595
(1/2,1/2,0)	M3+	(0,0,a)	P4/mbm (127)	1	0.9044

Global distortion: 1.6435 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative

displacements in this cell.

Irrep R4+

R4+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.031666	-0.000000
O3_2	0.000000	0.000000	0.063331

Irrep R5+

R5+ Mode La2 1

Atom	δx	δy	δz
La2	0.000000	0.000000	-0.089564

R5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.031666	0.000000
O3_2	0.000000	0.000000	0.063331

Irrep X5+

X5+ Mode La2 1

Atom	δx	δy	δz
La2	-0.089564	0.000000	0.000000

X5+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	-0.089564	0.000000	0.000000

Irrep M2+

M2+ Mode O3 1

Atom	δx	δy	δz
O3	-0.044782	0.000000	0.044782
O3_2	0.000000	0.000000	0.000000

Irrep M3+

M3+ Mode O3 1

Atom	δx	δy	δz
O3	-0.044782	0.000000	-0.044782
O3_2	0.000000	0.000000	0.000000

K-vector: R = (1/2,1/2,1/2)

Irrep: R4+

Direction: (a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1      0     -1 ] [      0]
[      0      2      0 ] [      0]
[      1      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{R4+}= 1.1945 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
-1.1945

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
La2	0.0000	0.0000	0.0000
O3	0.0000	-0.0317	0.0000
O3_2	0.0000	0.0000	-0.0633

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: R5+

Direction: (-a,a,0)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[      1       0       1  ] [       0]
[      0      -2       0  ] [       0]
[      1       0      -1  ] [       0]
```

The amplitude of this distortion is:
A_{R5+} = 0.0890 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

La2 1	O3 1
-0.9789	0.2041

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
La2	0.0000	0.0000	0.0877
O3	0.0000	-0.0065	0.0000
O3_2	0.0000	0.0000	0.0129

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: X = (0,1/2,0)

Irrep: X5+

Direction: (0,a,0,0,0,0)

Isotropy Subgroup: 63 Cmcm D2h-17

Transformation matrix:

```
[      1       1       0  ] [       0]
[      0       0      -2  ] [       0]
```

```
[     -1      1      0 ] [       0]
```

The amplitude of this distortion is:
A_{X5+} = 0.5649 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

La2 1	O3 1
-0.9685	-0.2490

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
La2	0.0867	-0.0000	-0.0000
O3	0.0000	0.0000	0.0000
O3_2	0.0223	-0.0000	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: M = (1/2,1/2,0)

Irrep: M2+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1      1      0 ] [     1/2]
[      0      0      1 ] [       0]
[      1     -1      0 ] [     1/2]
```

The amplitude of this distortion is:
A_{M2+} = 0.3595 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
0.3595

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
La2	0.0000	0.0000	0.0000
O3	-0.0448	0.0000	0.0448
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: M3+

Direction: (0,0,a)

Isotropy Subgroup: 127 P4/mbm D4h-5

Transformation matrix:

```
[      1       1       0 ] [       0]
[      0       0       1 ] [       0]
[      1      -1       0 ] [       0]
```

The amplitude of this distortion is:
A_{M3+} = 0.9044 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O3 1
0.9044

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Mn1	0.0000	0.0000	0.0000
La2	0.0000	0.0000	0.0000
O3	-0.0448	0.0000	-0.0448
O3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

NbS3

Ref: J. Rijnsdorp and F. Jellinek, J. Solid State Chem. 25, 325 (1978)

Symmetry mode analysis

High symmetry structure

```
11
4.963 3.365 9.144 90. 97.17 90.
4
Nb       1        2e       0.715500         0.750000         0.348650
S        1        2e       0.763400         0.250000         0.553550
S        2        2e       0.878850         0.250000         0.169450
S        3        2e       0.466950         0.250000         0.174150
```

Low symmetry structure

```
2
4.963 6.730 9.144 90. 97.17 90.
8
Nb       1        2i       0.715600         0.852600         0.350900
Nb       2        2i       0.715400         0.401300         0.346400
S        1        2i       0.763200         0.616300         0.561800
S        2        2i       0.763600         0.132700         0.545300
S        3        2i       0.874700         0.628800         0.155200
S        4        2i       0.883000         0.124800         0.183700
S        5        2i       0.463100         0.627400         0.161000
S        6        2i       0.470800         0.122400         0.187300
```

Transformation matrix

```
[      1      0      0 ] [       0]
[      0      2      0 ] [       0]
[      0      0      1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
002
4.963000 6.730000 9.144000 90.000000 97.169998 90.000000
8
Nb       1        2i       0.715500         0.375000         0.348650
Nb       1_2      2i       0.715500         0.875000         0.348650
S        1        2i       0.763400         0.125000         0.553550
S        1_2      2i       0.236600         0.375000         0.446450
S        2        2i       0.878850         0.125000         0.169450
S        2_2      2i       0.121150         0.375000         0.830550
S        3        2i       0.466950         0.125000         0.174150
S        3_2      2i       0.533050         0.375000         0.825850
```

Atom pairings and distances

Atom Mappings

WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2i	(x,y,z)	Nb1	(0.715500,0.375000,0.348650)	Nb2	(0.715400,0.401300,0.346400)
2i	(x,y,z)	Nb1_2	(0.715500,0.875000,0.348650)	Nb1	(0.715600,0.852600,0.350900)
2i	(x,y,z)	S1	(0.763400,0.125000,0.553550)	S2	(0.763600,0.132700,0.545300)
2i	(x,y,z)	S1_2	(0.236600,0.375000,0.446450)	S1	(0.236800,0.383700,0.438200)
2i	(x,y,z)	S2	(0.878850,0.125000,0.169450)	S4	(0.883000,0.124800,0.183700)
2i	(x,y,z)	S2_2	(0.121150,0.375000,0.830550)	S3	(0.125300,0.371200,0.844800)
2i	(x,y,z)	S3	(0.466950,0.125000,0.174150)	S6	(0.470800,0.122400,0.187300)
2i	(x,y,z)	S3_2	(0.533050,0.375000,0.825850)	S5	(0.536900,0.372600,0.839000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2i	(x,y,z)	Nb1	-0.0001	0.0263	-0.0022	0.1782
2i	(x,y,z)	Nb1_2	0.0001	-0.0224	0.0022	0.1521
2i	(x,y,z)	S1	0.0002	0.0077	-0.0083	0.0916
2i	(x,y,z)	S1_2	0.0002	0.0087	-0.0083	0.0956
2i	(x,y,z)	S2	0.0042	-0.0002	0.0143	0.1294
2i	(x,y,z)	S2_2	0.0042	-0.0038	0.0143	0.1319
2i	(x,y,z)	S3	0.0039	-0.0026	0.0132	0.1206
2i	(x,y,z)	S3_2	0.0039	-0.0024	0.0132	0.1205

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1782 Å
Total distortion amplitude: 0.5208 Å

Symmetry Modes Summary

Atoms	WP	Modes
Nb1 S3 S1 S2	2*e*	GM1+(2) GM2+(1) **Z1(3)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	P2_1/m (11)	8	0.0000
(0,0,0)	GM2+	(a)	P-1 (2)	4	0.0364

(0,1/2,0)	Z1	(0,a)	P-1 (2)	12	0.5195

Global distortion: 0.5208 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Nb1 1

Atom	δx	δy	δz
Nb1	0.000000	0.000000	-0.054681
Nb1_2	0.000000	0.000000	-0.054681

GM1+ Mode Nb1 2

Atom	δx	δy	δz
Nb1	-0.101540	0.000000	-0.006879
Nb1_2	-0.101540	0.000000	-0.006879

GM1+ Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.000000	0.054681
S1_2	0.000000	0.000000	-0.054681

GM1+ Mode S1 2

Atom	δx	δy	δz
S1	0.101540	-0.000000	0.006879
S1_2	-0.101540	0.000000	-0.006879

GM1+ Mode S2 1

Atom	δx	δy	δz
S2	0.000000	0.000000	0.054681
S2_2	0.000000	0.000000	-0.054681

GM1+ Mode S2 2

Atom	δx	δy	δz
S2	0.101540	-0.000000	0.006879
S2_2	-0.101540	0.000000	-0.006879

GM1+ Mode S3 1

Atom	δx	δy	δz
S3	0.000000	0.000000	0.054681
S3_2	0.000000	0.000000	-0.054681

GM1+ Mode S3 2

Atom	δx	δy	δz
S3	0.101540	-0.000000	0.006879
S3_2	-0.101540	0.000000	-0.006879

Irrep GM2+

GM2+ Mode Nb1 1

Atom	δx	δy	δz
Nb1	0.000000	-0.074294	0.000000
Nb1_2	0.000000	-0.074294	0.000000

GM2+ Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.074294	-0.000000
S1_2	0.000000	-0.074294	0.000000

GM2+ Mode S2 1

Atom	δx	δy	δz
S2	0.000000	0.074294	-0.000000
S2_2	0.000000	-0.074294	0.000000

GM2+ Mode S3 1

Atom	δx	δy	δz
S3	0.000000	0.074294	-0.000000
S3_2	0.000000	-0.074294	0.000000

Irrep Z1

Z1 Mode Nb1 1

Atom	δx	δy	δz
Nb1	0.000000	0.074294	-0.000000
Nb1_2	0.000000	-0.074294	0.000000

Z1 Mode Nb1 2

Atom	δx	δy	δz
Nb1	0.000000	0.000000	-0.054681
Nb1_2	0.000000	0.000000	0.054681

Z1 Mode Nb1 3

Atom	δx	δy	δz
Nb1	-0.101540	0.000000	-0.006879
Nb1_2	0.101540	-0.000000	0.006879

Z1 Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.074294	-0.000000
S1_2	0.000000	0.074294	-0.000000

Z1 Mode S1 2

Atom	δx	δy	δz
S1	0.000000	0.000000	-0.054681
S1_2	0.000000	0.000000	-0.054681

Z1 Mode S1 3

Atom	δx	δy	δz
S1	-0.101540	0.000000	-0.006879
S1_2	-0.101540	0.000000	-0.006879

Z1 Mode S2 1

Atom	δx	δy	δz
S2	0.000000	0.074294	-0.000000
S2_2	0.000000	0.074294	-0.000000

Z1 Mode S2 2

Atom	δx	δy	δz
S2	0.000000	0.000000	-0.054681
S2_2	0.000000	0.000000	-0.054681

Z1 Mode S2 3

Atom	δx	δy	δz
S2	-0.101540	0.000000	-0.006879
S2_2	-0.101540	0.000000	-0.006879

Z1 Mode S3 1

Atom	δx	δy	δz
S3	0.000000	0.074294	-0.000000
S3_2	0.000000	0.074294	-0.000000

Z1 Mode S3 2

Atom	δx	δy	δz
S3	0.000000	0.000000	-0.054681
S3_2	0.000000	0.000000	-0.054681

Z1 Mode S3 3

Atom	δx	δy	δz
S3	-0.101540	0.000000	-0.006879
S3_2	-0.101540	0.000000	-0.006879

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 11 P2_1/m C2h-2

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.0000 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Nb1 1	Nb1 2	S1 1	S1 2	S2 1	S2 2	S3 1	S3 2
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Nb1	0.0000	0.0000	0.0000
Nb1_2	0.0000	0.0000	0.0000

S1	0.0000	0.0000	0.0000
S1_2	0.0000	0.0000	0.0000
S2	0.0000	0.0000	0.0000
S2_2	0.0000	0.0000	0.0000
S3	0.0000	0.0000	0.0000
S3_2	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM2+

Direction: (a)

Isotropy Subgroup: 2 P-1 Ci-1

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM2+}= 0.0364 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Nb1 1	S1 1	S2 1	S3 1
-0.7216	-0.1850	0.6661	-0.0370

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Nb1	0.0000	0.0536	-0.0000
Nb1_2	0.0000	0.0536	-0.0000
S1	0.0000	-0.0137	0.0000
S1_2	0.0000	0.0137	-0.0000
S2	0.0000	0.0495	-0.0000
S2_2	0.0000	-0.0495	0.0000
S3	0.0000	-0.0027	0.0000
S3_2	0.0000	0.0027	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: Z = (0,1/2,0)

Irrep: Z1

Direction: (0,a)

Isotropy Subgroup: 2 P-1 Ci-1

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      2      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{Z1}= 0.5195 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Nb1 1	Nb1 2	Nb1 3	S1 1	S1 2	S1 3	S2 1	S2 2	S2 3	S3 1	S3 2	S3 3
0.6309	0.0790	0.0019	0.2124	0.2909	-0.0038	-0.0518	-0.4917	-0.0787	-0.0648	-0.4537	-0.0730

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Nb1	-0.0002	0.0469	-0.0043
Nb1_2	0.0002	-0.0469	0.0043
S1	0.0004	0.0158	-0.0159
S1_2	0.0004	0.0158	-0.0159
S2	0.0080	-0.0039	0.0274
S2_2	0.0080	-0.0039	0.0274
S3	0.0074	-0.0048	0.0253
S3_2	0.0074	-0.0048	0.0253

Virtual structure with only this symmetry component of the distortion frozen.

K2SeO4 lock-in threefold phase

Ref: Yamada, N.;Ono, Y.;Ikeda, T. , Journal of the Physical Society of Japan (1984) 53, 2565-2574

Symmetry mode analysis

High symmetry structure

```
62
7.6610 6.0030 10.4660 90.00 90.00 90.00
6
Se       1       4c      0.222220        0.250000        0.581330
K        1       4c      0.167020        0.250000        0.919110
K        2       4c      0.998280        0.250000        0.292460
O        1       8d      0.289120        0.027690        0.658660
O        2       4c      0.312050        0.250000        0.438310
O        3       4c      0.009250        0.250000        0.570950
```

Low symmetry structure

```
33
22.716 10.339 5.967 90. 90. 90.
21
K        1       4a      0.054400        0.079990        0.255600
K        2       4a      0.388980        0.079740        0.244070
K        3       4a      0.722480        0.081080        0.229560
K        4       4a      -0.000080       0.708040        0.270400
K        5       4a      0.332740        0.705950        0.234430
K        6       4a      0.666430        0.708140        0.249920
Se       1       4a      0.074010        0.417110        0.243650
Se       2       4a      0.406560        0.417990        0.260630
Se       3       4a      0.741560        0.420320        0.243070
O        1       4a      0.101800        0.348600        0.037300
O        2       4a      0.424700        0.340000        0.031400
O        3       4a      0.754500        0.329100        0.027800
O        4       4a      0.094200        0.335800        0.466000
O        5       4a      0.432400        0.339300        0.488800
O        6       4a      0.771500        0.351800        0.480700
O        7       4a      0.101200        0.567800        0.260800
O        8       4a      0.441100        0.556200        0.253900
O        9       4a      0.771700        0.561800        0.204900
O        10      4a      0.002400        0.431100        0.222300
O        11      4a      0.338600        0.433100        0.295200
O        12      4a      0.669300        0.429500        0.279900
```

Transformation matrix

```
[     3     0     0 ] [       0]
[     0     0     1 ] [       0]
[     0    -1     0 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
033
22.983000 10.466000 6.003000 90.000000 90.000000 90.000000
21
Se       1       4a      0.074073        0.418670        0.250000
Se       1_2     4a      0.092593        0.918670        0.750000
Se       1_3     4a      0.240740        0.081330        0.250000
K        1       4a      0.055673        0.080890        0.250000
K        1_2     4a      0.110993        0.580890        0.750000
K        1_3     4a      0.222340        0.419110        0.250000
K        2       4a      0.332760        0.707540        0.250000
K        2_2     4a      0.833907        0.207540        0.750000
K        2_3     4a      0.499427        0.792460        0.250000
O        1       4a      0.096373        0.341340        0.027690
O        1_2     4a      0.070293        0.841340        0.972310
O        1_3     4a      0.263040        0.158660        0.472310
O        1_4     4a      0.903627        0.658660        0.972310
O        1_5     4a      0.263040        0.158660        0.027690
O        1_6     4a      0.070293        0.841340        0.527690
O        2       4a      0.104017        0.561690        0.250000
O        2_2     4a      0.062650        0.061690        0.750000
O        2_3     4a      0.270683        0.938310        0.250000
O        3       4a      0.003083        0.429050        0.250000
O        3_2     4a      0.163583        0.929050        0.750000
O        3_3     4a      0.169750        0.070950        0.250000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4a	(x,y,z)	Se1	(0.074073,0.418670,0.250000)	Se1	(0.074010,0.417110,0.243650)
4a	(x,y,z)	Se1_2	(0.092593,0.918670,0.750000)	Se2	(0.093440,0.917990,0.760630)
4a	(x,y,z)	Se1_3	(0.240740,0.081330,0.250000)	Se3	(0.241560,0.079680,0.243070)
4a	(x,y,z)	K1	(0.055673,0.080890,0.250000)	K1	(0.054400,0.079990,0.255600)
4a	(x,y,z)	K1_2	(0.110993,0.580890,0.750000)	K2	(0.111020,0.579740,0.744070)

4a	(x,y,z)	K1_3	(0.222340,0.419110,0.250000)	K3	(0.222480,0.418920,0.229560)
4a	(x,y,z)	K2	(0.332760,0.707540,0.250000)	K5	(0.332740,0.705950,0.234430)
4a	(x,y,z)	K2_2	(0.833907,0.207540,0.750000)	K6	(0.833570,0.208140,0.749920)
4a	(x,y,z)	K2_3	(0.499427,0.792460,0.250000)	K4	(0.499920,0.791960,0.270400)
4a	(x,y,z)	O1	(0.096373,0.341340,0.027690)	O1	(0.101800,0.348600,0.037300)
4a	(x,y,z)	O1_2	(0.070293,0.841340,0.972310)	O5	(0.067600,0.839300,0.988800)
4a	(x,y,z)	O1_3	(0.263040,0.158660,0.472310)	O6	(0.271500,0.148200,0.480700)
4a	(x,y,z)	O1_4	(0.903627,0.658660,0.972310)	O4	(0.905800,0.664200,0.966000)
4a	(x,y,z)	O1_5	(0.263040,0.158660,0.027690)	O3	(0.254500,0.170900,0.027800)
4a	(x,y,z)	O1_6	(0.070293,0.841340,0.527690)	O2	(0.075300,0.840000,0.531400)
4a	(x,y,z)	O2	(0.104017,0.561690,0.250000)	O7	(0.101200,0.567800,0.260800)
4a	(x,y,z)	O2_2	(0.062650,0.061690,0.750000)	O8	(0.058900,0.056200,0.753900)
4a	(x,y,z)	O2_3	(0.270683,0.938310,0.250000)	O9	(0.271700,0.938200,0.204900)
4a	(x,y,z)	O3	(0.003083,0.429050,0.250000)	O10	(0.002400,0.431100,0.222300)
4a	(x,y,z)	O3_2	(0.163583,0.929050,0.750000)	O11	(0.161400,0.933100,0.795200)
4a	(x,y,z)	O3_3	(0.169750,0.070950,0.250000)	O12	(0.169300,0.070500,0.279900)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4a	(x,y,z)	Se1	-0.0001	-0.0016	-0.0063	0.0415
4a	(x,y,z)	Se1_2	0.0008	-0.0007	0.0106	0.0671
4a	(x,y,z)	Se1_3	0.0008	-0.0016	-0.0069	0.0488
4a	(x,y,z)	K1	-0.0013	-0.0009	0.0056	0.0456
4a	(x,y,z)	K1_2	0.0000	-0.0011	-0.0059	0.0376
4a	(x,y,z)	K1_3	0.0001	-0.0002	-0.0204	0.1228
4a	(x,y,z)	K2	-0.0000	-0.0016	-0.0156	0.0949
4a	(x,y,z)	K2_2	-0.0003	0.0006	-0.0001	0.0100
4a	(x,y,z)	K2_3	0.0005	-0.0005	0.0204	0.1231
4a	(x,y,z)	O1	0.0054	0.0073	0.0096	0.1570
4a	(x,y,z)	O1_2	-0.0027	-0.0020	0.0165	0.1187
4a	(x,y,z)	O1_3	0.0085	-0.0105	0.0084	0.2288
4a	(x,y,z)	O1_4	0.0022	0.0055	-0.0063	0.0854
4a	(x,y,z)	O1_5	-0.0085	0.0122	0.0001	0.2344
4a	(x,y,z)	O1_6	0.0050	-0.0013	0.0037	0.1180
4a	(x,y,z)	O2	-0.0028	0.0061	0.0108	0.1117
4a	(x,y,z)	O2_2	-0.0037	-0.0055	0.0039	0.1062
4a	(x,y,z)	O2_3	0.0010	-0.0001	-0.0451	0.2717
4a	(x,y,z)	O3	-0.0007	0.0021	-0.0277	0.1684
4a	(x,y,z)	O3_2	-0.0022	0.0040	0.0452	0.2792
4a	(x,y,z)	O3_3	-0.0004	-0.0004	0.0299	0.1798

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2792 Å
Total distortion amplitude: 1.3489 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, 0.00144)

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
4a	(x,y,z)	Se1	(0.074073,0.418670,0.250000)	Se1	(0.074010,0.417110,0.242206)
4a	(x,y,z)	Se1_2	(0.092593,0.918670,0.750000)	Se2	(0.093440,0.917990,0.759186)
4a	(x,y,z)	Se1_3	(0.240740,0.081330,0.250000)	Se3	(0.241560,0.079680,0.241626)
4a	(x,y,z)	K1	(0.055673,0.080890,0.250000)	K1	(0.054400,0.079990,0.254156)
4a	(x,y,z)	K1_2	(0.110993,0.580890,0.750000)	K2	(0.111020,0.579740,0.742626)
4a	(x,y,z)	K1_3	(0.222340,0.419110,0.250000)	K3	(0.222480,0.418920,0.228116)

4a	(x,y,z)	K2	(0.332760,0.707540,0.250000)	K5	(0.332740,0.705950,0.232986)
4a	(x,y,z)	K2_2	(0.833907,0.207540,0.750000)	K6	(0.833570,0.208140,0.748476)
4a	(x,y,z)	K2_3	(0.499427,0.792460,0.250000)	K4	(0.499920,0.791960,0.268956)
4a	(x,y,z)	O1	(0.096373,0.341340,0.027690)	O1	(0.101800,0.348600,0.035856)
4a	(x,y,z)	O1_2	(0.070293,0.841340,0.972310)	O5	(0.067600,0.839300,0.987356)
4a	(x,y,z)	O1_3	(0.263040,0.158660,0.472310)	O6	(0.271500,0.148200,0.479256)
4a	(x,y,z)	O1_4	(0.903627,0.658660,0.972310)	O4	(0.905800,0.664200,0.964556)
4a	(x,y,z)	O1_5	(0.263040,0.158660,0.027690)	O3	(0.254500,0.170900,0.026356)
4a	(x,y,z)	O1_6	(0.070293,0.841340,0.527690)	O2	(0.075300,0.840000,0.529956)
4a	(x,y,z)	O2	(0.104017,0.561690,0.250000)	O7	(0.101200,0.567800,0.259356)
4a	(x,y,z)	O2_2	(0.062650,0.061690,0.750000)	O8	(0.058900,0.056200,0.752456)
4a	(x,y,z)	O2_3	(0.270683,0.938310,0.250000)	O9	(0.271700,0.938200,0.203456)
4a	(x,y,z)	O3	(0.003083,0.429050,0.250000)	O10	(0.002400,0.431100,0.220856)
4a	(x,y,z)	O3_2	(0.163583,0.929050,0.750000)	O11	(0.161400,0.933100,0.793756)
4a	(x,y,z)	O3_3	(0.169750,0.070950,0.250000)	O12	(0.169300,0.070500,0.278456)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4a	(x,y,z)	Se1	-0.0001	-0.0016	-0.0078	0.0496
4a	(x,y,z)	Se1_2	0.0008	-0.0007	0.0092	0.0589
4a	(x,y,z)	Se1_3	0.0008	-0.0016	-0.0084	0.0564
4a	(x,y,z)	K1	-0.0013	-0.0009	0.0042	0.0396
4a	(x,y,z)	K1_2	0.0000	-0.0011	-0.0074	0.0459
4a	(x,y,z)	K1_3	0.0001	-0.0002	-0.0219	0.1314
4a	(x,y,z)	K2	-0.0000	-0.0016	-0.0170	0.1035
4a	(x,y,z)	K2_2	-0.0003	0.0006	-0.0015	0.0135
4a	(x,y,z)	K2_3	0.0005	-0.0005	0.0190	0.1145
4a	(x,y,z)	O1	0.0054	0.0073	0.0082	0.1541
4a	(x,y,z)	O1_2	-0.0027	-0.0020	0.0150	0.1116
4a	(x,y,z)	O1_3	0.0085	-0.0105	0.0069	0.2270
4a	(x,y,z)	O1_4	0.0022	0.0055	-0.0078	0.0896
4a	(x,y,z)	O1_5	-0.0085	0.0122	-0.0013	0.2345
4a	(x,y,z)	O1_6	0.0050	-0.0013	0.0023	0.1167
4a	(x,y,z)	O2	-0.0028	0.0061	0.0094	0.1069
4a	(x,y,z)	O2_2	-0.0037	-0.0055	0.0025	0.1046
4a	(x,y,z)	O2_3	0.0010	-0.0001	-0.0465	0.2804
4a	(x,y,z)	O3	-0.0007	0.0021	-0.0291	0.1770
4a	(x,y,z)	O3_2	-0.0022	0.0040	0.0438	0.2708
4a	(x,y,z)	O3_3	-0.0004	-0.0004	0.0285	0.1712

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2804 Å
Total distortion amplitude: 1.3467 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	8*d*	GM1+(3) GM4-(3) **SM2(6)** SM3(6)
Se1 O3 K2 K1 O2	4*c*	GM1+(2) GM4-(1) **SM2(2)** SM3(4)

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Pnma (62)	13	0.1165
(0,0,0)	GM4-	(a)	Pna2_1 (33)	8	0.5495

(1/3,0,0)	SM2	(a,0)	Pna2_1 (33)	16	1.1597
(1/3,0,0)	SM3	(a,0)	Pnma (62)	26	0.3910

Global distortion: 1.3466 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode Se1 1

Atom	δx	δy	δz
Se1	0.000000	-0.027582	0.000000
Se1_2	0.000000	-0.027582	0.000000
Se1_3	0.000000	0.027582	-0.000000

GM1+ Mode Se1 2

Atom	δx	δy	δz
Se1	0.012560	-0.000000	-0.000000
Se1_2	-0.012560	0.000000	0.000000
Se1_3	0.012560	-0.000000	-0.000000

GM1+ Mode K1 1

Atom	δx	δy	δz
K1	0.000000	-0.027582	0.000000
K1_2	0.000000	-0.027582	0.000000
K1_3	0.000000	0.027582	-0.000000

GM1+ Mode K1 2

Atom	δx	δy	δz
K1	0.012560	-0.000000	-0.000000
K1_2	-0.012560	0.000000	0.000000
K1_3	0.012560	-0.000000	-0.000000

GM1+ Mode K2 1

Atom	δx	δy	δz
K2	0.000000	-0.027582	0.000000
K2_2	0.000000	-0.027582	0.000000
K2_3	0.000000	0.027582	-0.000000

GM1+ Mode K2 2

Atom	δx	δy	δz
K2	0.012560	-0.000000	-0.000000
K2_2	-0.012560	0.000000	0.000000
K2_3	0.012560	-0.000000	-0.000000

GM1+ Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.019504	0.000000
O1_2	0.000000	-0.019504	0.000000
O1_3	0.000000	0.019504	-0.000000
O1_4	0.000000	0.019504	-0.000000
O1_5	0.000000	0.019504	-0.000000
O1_6	0.000000	-0.019504	0.000000

GM1+ Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.034004
O1_2	0.000000	0.000000	-0.034004
O1_3	0.000000	0.000000	-0.034004
O1_4	0.000000	0.000000	-0.034004

O1_5	0.000000	0.000000	0.034004
O1_6	0.000000	0.000000	0.034004

GM1+ Mode O1 3

Atom	δx	δy	δz
O1	0.008882	-0.000000	-0.000000
O1_2	-0.008882	0.000000	0.000000
O1_3	0.008882	-0.000000	-0.000000
O1_4	-0.008882	0.000000	0.000000
O1_5	0.008882	-0.000000	-0.000000
O1_6	-0.008882	0.000000	0.000000

GM1+ Mode O2 1

Atom	δx	δy	δz
O2	0.000000	-0.027582	0.000000
O2_2	0.000000	-0.027582	0.000000
O2_3	0.000000	0.027582	-0.000000

GM1+ Mode O2 2

Atom	δx	δy	δz
O2	0.012560	-0.000000	-0.000000
O2_2	-0.012560	0.000000	0.000000
O2_3	0.012560	-0.000000	-0.000000

GM1+ Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.027582	0.000000
O3_2	0.000000	-0.027582	0.000000
O3_3	0.000000	0.027582	-0.000000

GM1+ Mode O3 2

Atom	δx	δy	δz
O3	0.012560	-0.000000	-0.000000
O3_2	-0.012560	0.000000	0.000000
O3_3	0.012560	-0.000000	-0.000000

Irrep GM4-

GM4- Mode Se1 1

Atom	δx	δy	δz
Se1	0.000000	0.000000	0.048088
Se1_2	0.000000	0.000000	0.048088
Se1_3	0.000000	0.000000	0.048088

GM4- Mode K1 1

Atom	δx	δy	δz
K1	0.000000	0.000000	0.048088
K1_2	0.000000	0.000000	0.048088
K1_3	0.000000	0.000000	0.048088

GM4- Mode K2 1

Atom	δx	δy	δz
K2	0.000000	0.000000	0.048088
K2_2	0.000000	0.000000	0.048088
K2_3	0.000000	0.000000	0.048088

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.008882	-0.000000	-0.000000

O1_2	0.008882	-0.000000	-0.000000
O1_3	-0.008882	0.000000	0.000000
O1_4	0.008882	-0.000000	-0.000000
O1_5	0.008882	-0.000000	-0.000000
O1_6	-0.008882	0.000000	0.000000

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.034004
O1_2	0.000000	0.000000	0.034004
O1_3	0.000000	0.000000	0.034004
O1_4	0.000000	0.000000	0.034004
O1_5	0.000000	0.000000	0.034004
O1_6	0.000000	0.000000	0.034004

GM4- Mode O1 3

Atom	δx	δy	δz
O1	0.000000	-0.019504	0.000000
O1_2	0.000000	0.019504	-0.000000
O1_3	0.000000	-0.019504	0.000000
O1_4	0.000000	-0.019504	0.000000
O1_5	0.000000	0.019504	-0.000000
O1_6	0.000000	-0.019504	0.000000

GM4- Mode O2 1

Atom	δx	δy	δz
O2	0.000000	0.000000	0.048088
O2_2	0.000000	0.000000	0.048088
O2_3	0.000000	0.000000	0.048088

GM4- Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.048088
O3_2	0.000000	0.000000	0.048088
O3_3	0.000000	0.000000	0.048088

Irrep SM2

SM2 Mode Se1 1

Atom	δx	δy	δz
Se1	0.000000	0.000000	0.068007
Se1_2	0.000000	0.000000	-0.034004
Se1_3	0.000000	0.000000	-0.034004

SM2 Mode Se1 2

Atom	δx	δy	δz
Se1	0.000000	0.000000	0.000000
Se1_2	0.000000	0.000000	0.058896
Se1_3	0.000000	0.000000	-0.058896

SM2 Mode K1 1

Atom	δx	δy	δz
K1	0.000000	0.000000	0.068007
K1_2	0.000000	0.000000	-0.034004
K1_3	0.000000	0.000000	-0.034004

SM2 Mode K1 2

Atom	δx	δy	δz
K1	0.000000	0.000000	0.000000

K1_2	0.000000	0.000000	0.058896
K1_3	0.000000	0.000000	-0.058896

SM2 Mode K2 1

Atom	δx	δy	δz
K2	0.000000	0.000000	0.000000
K2_2	0.000000	0.000000	0.058896
K2_3	0.000000	0.000000	-0.058896

SM2 Mode K2 2

Atom	δx	δy	δz
K2	0.000000	0.000000	0.068007
K2_2	0.000000	0.000000	-0.034004
K2_3	0.000000	0.000000	-0.034004

SM2 Mode O1 1

Atom	δx	δy	δz
O1	0.012560	-0.000000	-0.000000
O1_2	-0.006280	0.000000	0.000000
O1_3	0.006280	-0.000000	-0.000000
O1_4	0.012560	-0.000000	-0.000000
O1_5	-0.006280	0.000000	0.000000
O1_6	0.006280	-0.000000	-0.000000

SM2 Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.048088
O1_2	0.000000	0.000000	-0.024044
O1_3	0.000000	0.000000	-0.024044
O1_4	0.000000	0.000000	0.048088
O1_5	0.000000	0.000000	-0.024044
O1_6	0.000000	0.000000	-0.024044

SM2 Mode O1 3

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.010878	-0.000000	-0.000000
O1_3	0.010878	-0.000000	-0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	-0.010878	0.000000	0.000000
O1_6	-0.010878	0.000000	0.000000

SM2 Mode O1 4

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.023887	-0.000000
O1_3	0.000000	0.023887	-0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	-0.023887	0.000000
O1_6	0.000000	-0.023887	0.000000

SM2 Mode O1 5

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	0.041646
O1_3	0.000000	0.000000	-0.041646
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.000000	-0.041646

O1_6	0.000000	0.000000	0.041646

SM2 Mode O1 6

Atom	δx	δy	δz
O1	0.000000	-0.027582	0.000000
O1_2	0.000000	-0.013791	0.000000
O1_3	0.000000	0.013791	-0.000000
O1_4	0.000000	-0.027582	0.000000
O1_5	0.000000	-0.013791	0.000000
O1_6	0.000000	0.013791	-0.000000

SM2 Mode O2 1

Atom	δx	δy	δz
O2	0.000000	0.000000	0.068007
O2_2	0.000000	0.000000	-0.034004
O2_3	0.000000	0.000000	-0.034004

SM2 Mode O2 2

Atom	δx	δy	δz
O2	0.000000	0.000000	0.000000
O2_2	0.000000	0.000000	0.058896
O2_3	0.000000	0.000000	-0.058896

SM2 Mode O3 1

Atom	δx	δy	δz
O3	0.000000	0.000000	0.068007
O3_2	0.000000	0.000000	-0.034004
O3_3	0.000000	0.000000	-0.034004

SM2 Mode O3 2

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	0.000000	0.058896
O3_3	0.000000	0.000000	-0.058896

Irrep SM3

SM3 Mode Se1 1

Atom	δx	δy	δz
Se1	0.000000	-0.039007	0.000000
Se1_2	0.000000	0.019504	-0.000000
Se1_3	0.000000	-0.019504	0.000000

SM3 Mode Se1 2

Atom	δx	δy	δz
Se1	0.000000	0.000000	0.000000
Se1_2	0.000000	-0.033781	0.000000
Se1_3	0.000000	-0.033781	0.000000

SM3 Mode Se1 3

Atom	δx	δy	δz
Se1	0.000000	0.000000	0.000000
Se1_2	-0.015383	0.000000	0.000000
Se1_3	-0.015383	0.000000	0.000000

SM3 Mode Se1 4

Atom	δx	δy	δz
Se1	0.017763	-0.000000	-0.000000
Se1_2	0.008882	-0.000000	-0.000000

Se1_3	-0.008882	0.000000	0.000000

SM3 Mode K1 1

Atom	δx	δy	δz
K1	0.000000	-0.039007	0.000000
K1_2	0.000000	0.019504	-0.000000
K1_3	0.000000	-0.019504	0.000000

SM3 Mode K1 2

Atom	δx	δy	δz
K1	0.000000	0.000000	0.000000
K1_2	0.000000	-0.033781	0.000000
K1_3	0.000000	-0.033781	0.000000

SM3 Mode K1 3

Atom	δx	δy	δz
K1	0.000000	0.000000	0.000000
K1_2	-0.015383	0.000000	0.000000
K1_3	-0.015383	0.000000	0.000000

SM3 Mode K1 4

Atom	δx	δy	δz
K1	0.017763	-0.000000	-0.000000
K1_2	0.008882	-0.000000	-0.000000
K1_3	-0.008882	0.000000	0.000000

SM3 Mode K2 1

Atom	δx	δy	δz
K2	0.017763	-0.000000	-0.000000
K2_2	0.008882	-0.000000	-0.000000
K2_3	-0.008882	0.000000	0.000000

SM3 Mode K2 2

Atom	δx	δy	δz
K2	0.000000	-0.039007	0.000000
K2_2	0.000000	0.019504	-0.000000
K2_3	0.000000	-0.019504	0.000000

SM3 Mode K2 3

Atom	δx	δy	δz
K2	0.000000	0.000000	0.000000
K2_2	0.000000	-0.033781	0.000000
K2_3	0.000000	-0.033781	0.000000

SM3 Mode K2 4

Atom	δx	δy	δz
K2	0.000000	0.000000	0.000000
K2_2	-0.015383	0.000000	0.000000
K2_3	-0.015383	0.000000	0.000000

SM3 Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.027582	0.000000
O1_2	0.000000	0.013791	-0.000000
O1_3	0.000000	-0.013791	0.000000
O1_4	0.000000	0.027582	-0.000000
O1_5	0.000000	-0.013791	0.000000
O1_6	0.000000	0.013791	-0.000000

SM3 Mode O1 2

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	0.000000	-0.041646
O1_3	0.000000	0.000000	0.041646
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	0.000000	-0.041646
O1_6	0.000000	0.000000	0.041646

SM3 Mode O1 3

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	0.000000	-0.023887	0.000000
O1_3	0.000000	-0.023887	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	0.000000	-0.023887	0.000000
O1_6	0.000000	-0.023887	0.000000

SM3 Mode O1 4

Atom	δx	δy	δz
O1	0.000000	0.000000	0.000000
O1_2	-0.010878	0.000000	0.000000
O1_3	-0.010878	0.000000	0.000000
O1_4	0.000000	0.000000	0.000000
O1_5	-0.010878	0.000000	0.000000
O1_6	-0.010878	0.000000	0.000000

SM3 Mode O1 5

Atom	δx	δy	δz
O1	0.000000	0.000000	0.048088
O1_2	0.000000	0.000000	0.024044
O1_3	0.000000	0.000000	0.024044
O1_4	0.000000	0.000000	-0.048088
O1_5	0.000000	0.000000	-0.024044
O1_6	0.000000	0.000000	-0.024044

SM3 Mode O1 6

Atom	δx	δy	δz
O1	0.012560	-0.000000	-0.000000
O1_2	0.006280	-0.000000	-0.000000
O1_3	-0.006280	0.000000	0.000000
O1_4	-0.012560	0.000000	0.000000
O1_5	-0.006280	0.000000	0.000000
O1_6	0.006280	-0.000000	-0.000000

SM3 Mode O2 1

Atom	δx	δy	δz
O2	0.000000	-0.039007	0.000000
O2_2	0.000000	0.019504	-0.000000
O2_3	0.000000	-0.019504	0.000000

SM3 Mode O2 2

Atom	δx	δy	δz
O2	0.000000	0.000000	0.000000
O2_2	0.000000	-0.033781	0.000000
O2_3	0.000000	-0.033781	0.000000

SM3 Mode O2 3

Atom	δx	δy	δz

O2	0.000000	0.000000	0.000000
O2_2	-0.015383	0.000000	0.000000
O2_3	-0.015383	0.000000	0.000000

SM3 Mode O2 4

Atom	δx	δy	δz
O2	0.017763	-0.000000	-0.000000
O2_2	0.008882	-0.000000	-0.000000
O2_3	-0.008882	0.000000	0.000000

SM3 Mode O3 1

Atom	δx	δy	δz
O3	0.000000	-0.039007	0.000000
O3_2	0.000000	0.019504	-0.000000
O3_3	0.000000	-0.019504	0.000000

SM3 Mode O3 2

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	0.000000	-0.033781	0.000000
O3_3	0.000000	-0.033781	0.000000

SM3 Mode O3 3

Atom	δx	δy	δz
O3	0.000000	0.000000	0.000000
O3_2	-0.015383	0.000000	0.000000
O3_3	-0.015383	0.000000	0.000000

SM3 Mode O3 4

Atom	δx	δy	δz
O3	0.017763	-0.000000	-0.000000
O3_2	0.008882	-0.000000	-0.000000
O3_3	-0.008882	0.000000	0.000000

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+} = 0.1165 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Se1 1	Se1 2	K1 1	K1 2	K2 1	K2 2	O1 1	O1 2	O1 3	O2 1	O2 2	O3 1	O3 2
0.0612	-0.0205	0.1930	-0.2643	0.0508	0.1846	0.2524	-0.2163	0.1386	-0.0757	0.4443	-0.6797	0.2393

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Se1	-0.0003	-0.0017	0.0000
Se1_2	0.0003	-0.0017	0.0000
Se1_3	-0.0003	0.0017	-0.0000
K1	-0.0033	-0.0053	0.0000
K1_2	0.0033	-0.0053	-0.0000

K1_3	-0.0033	0.0053	0.0000
K2	0.0023	-0.0014	-0.0000
K2_2	-0.0023	-0.0014	0.0000
K2_3	0.0023	0.0014	-0.0000
O1	0.0012	-0.0049	-0.0074
O1_2	-0.0012	-0.0049	0.0074
O1_3	0.0012	0.0049	0.0074
O1_4	-0.0012	0.0049	0.0074
O1_5	0.0012	0.0049	-0.0074
O1_6	-0.0012	-0.0049	-0.0074
O2	0.0056	0.0021	-0.0000
O2_2	-0.0056	0.0021	0.0000
O2_3	0.0056	-0.0021	-0.0000
O3	0.0030	0.0187	-0.0000
O3_2	-0.0030	0.0187	-0.0000
O3_3	0.0030	-0.0187	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: GM4-

Direction: (a)

Isotropy Subgroup: 33 Pna2_1 C2v-9

Transformation matrix:

```
[      1      0      0 ] [       0]
[      0      0     -1 ] [       0]
[      0      1      0 ] [       0]
```

The amplitude of this distortion is:
A_{GM4-} = 0.5495 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Se1 1	K1 1	K2 1	O1 1	O1 2	O1 3	O2 1	O3 1
-0.0881	-0.3167	0.0053	-0.5840	0.2082	0.1431	-0.4381	0.5433

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Se1	0.0000	0.0000	-0.0042
Se1_2	0.0000	0.0000	-0.0042
Se1_3	0.0000	0.0000	-0.0042
K1	0.0000	0.0000	-0.0152
K1_2	0.0000	0.0000	-0.0152
K1_3	0.0000	0.0000	-0.0152
K2	0.0000	0.0000	0.0003
K2_2	0.0000	0.0000	0.0003
K2_3	0.0000	0.0000	0.0003
O1	-0.0052	-0.0028	0.0071
O1_2	-0.0052	0.0028	0.0071
O1_3	0.0052	-0.0028	0.0071
O1_4	-0.0052	-0.0028	0.0071
O1_5	-0.0052	0.0028	0.0071
O1_6	0.0052	-0.0028	0.0071
O2	0.0000	0.0000	-0.0211
O2_2	0.0000	0.0000	-0.0211
O2_3	0.0000	0.0000	-0.0211
O3	0.0000	0.0000	0.0261

O3_2	0.0000	0.0000	0.0261
O3_3	0.0000	0.0000	0.0261

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: SM = (1/3,0,0)

Irrep: SM2

Direction: (a,0)

Isotropy Subgroup: 33 Pna2_1 C2v-9

Transformation matrix:

```
[      3      0      0 ] [       0]
[      0      0      1 ] [       0]
[      0     -1      0 ] [       0]
```

The amplitude of this distortion is:
A_{SM2}= 1.1597 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Se1 1	Se1 2	K1 1	K1 2	K2 1	K2 2	O1 1	O1 2	O1 3	O1 4	O1 5	O1 6	O2 1	O2 2	O3 1	O3 2
-0.0693	0.1285	0.1588	0.1062	-0.1499	-0.2175	0.4565	-0.0660	0.1843	-0.2112	0.0606	-0.2480	0.2654	0.3587	-0.5515	0.1120

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Se1	0.0000	0.0000	-0.0047
Se1_2	0.0000	0.0000	0.0099
Se1_3	0.0000	0.0000	-0.0052
K1	0.0000	0.0000	0.0108
K1_2	0.0000	0.0000	0.0009
K1_3	0.0000	0.0000	-0.0117
K2	0.0000	0.0000	-0.0148
K2_2	0.0000	0.0000	-0.0014
K2_3	0.0000	0.0000	0.0162
O1	0.0057	0.0068	-0.0032
O1_2	-0.0009	-0.0016	0.0041
O1_3	0.0049	-0.0085	-0.0009
O1_4	0.0057	0.0068	-0.0032
O1_5	-0.0049	0.0085	-0.0009
O1_6	0.0009	0.0016	0.0041
O2	0.0000	0.0000	0.0181
O2_2	0.0000	0.0000	0.0121
O2_3	0.0000	0.0000	-0.0302
O3	0.0000	0.0000	-0.0375
O3_2	0.0000	0.0000	0.0254
O3_3	0.0000	0.0000	0.0122

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: SM3

Direction: (a,0)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      3      0      0 ] [       0]
[      0      1      0 ] [       0]
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{SM3}= 0.3910 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Se1 1	Se1 2	Se1 3	Se1 4	K1 1	K1 2	K1 3	K1 4	K2 1	K2 2	K2 3	K2 4	O1 1	O1 2	O1 3	O1 4	O1 5	O1 6	O2 1
0.0894	0.0882	-0.1386	-0.0048	0.0184	0.0507	-0.0139	-0.1276	-0.0418	0.0935	-0.0038	-0.0130	-0.1329	-0.0691	0.0428	-0.1313	0.4689	0.3021	-0.3846

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Se1	-0.0001	-0.0035	0.0000
Se1_2	0.0021	-0.0012	-0.0000
Se1_3	0.0022	-0.0047	-0.0000
K1	-0.0023	-0.0007	0.0000
K1_2	-0.0009	-0.0014	0.0000
K1_3	0.0013	-0.0021	-0.0000
K2	-0.0007	-0.0036	0.0000
K2_2	-0.0002	0.0020	-0.0000
K2_3	0.0006	-0.0017	0.0000
O1	0.0038	0.0037	0.0225
O1_2	0.0033	-0.0029	0.0142
O1_3	-0.0005	0.0008	0.0084
O1_4	-0.0038	-0.0037	-0.0225
O1_5	-0.0005	0.0008	-0.0084
O1_6	0.0033	-0.0029	-0.0142
O2	-0.0089	0.0150	0.0000
O2_2	-0.0079	-0.0147	0.0000
O2_3	0.0009	0.0003	-0.0000
O3	-0.0026	-0.0003	0.0000
O3_2	-0.0047	0.0048	0.0000
O3_3	-0.0020	0.0044	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Thiourea

Ref: S. Tanisaki, H. Mashiyama, K. Hasebe, Acta Cryst. B44 (1988) 441-445

Symmetry mode analysis

High symmetry structure

```
62
7.545 8.54078 5.467 90 90 90
3
S       1       4c      -0.007600       0.250000        0.114730
C       1       4c      0.088120        0.250000        -0.167720
N       1       8d      0.127540        0.382770        -0.279820
```

Low symmetry structure

```
62
7.5450 76.8670 5.4670 90.00 90.00 90.00
19
S       1       4c      0.025300        0.250000        0.101600
S       2       8d      0.021700        0.361030        0.102800
S       3       8d      -0.000400       0.472240        0.113900
S       4       8d      -0.028000       0.583290        0.122800
S       5       8d      -0.042600       0.694330        0.125300
C       1       4c      0.102400        0.250000        -0.194000
C       2       8d      0.098500        0.361100        -0.192100
C       3       8d      0.093900        0.472560        -0.174200
C       4       8d      0.082800        0.583560        -0.152000
C       5       8d      0.076100        0.694570        -0.143600
N       1       8d      0.130500        0.264760        -0.312100
N       2       8d      0.129500        0.346570        -0.309900
N       3       8d      0.127300        0.376160        -0.308700
N       4       8d      0.130200        0.457900        -0.291200
N       5       8d      0.130600        0.487450        -0.284100
N       6       8d      0.129300        0.568830        -0.257800
N       7       8d      0.127400        0.598380        -0.255500
N       8       8d      0.122500        0.679660        -0.250800
N       9       8d      0.123600        0.709310        -0.245500
```

Transformation matrix

```
[      1      0      0 ] [       0]
[      0      9      0 ] [       0]
[      0      0      1 ] [       0]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
062
7.545000 76.867020 5.467000 90.000000 90.000000 90.000000
19
S       1       8d      0.992400        0.027778        0.114730
S       1_2     8d      0.007600        0.083333        0.885270
S       1_3     8d      0.992400        0.138889        0.114730
S       1_4     4c      0.992400        0.250000        0.114730
S       1_5     8d      0.992400        0.694444        0.114730
```

C	1	8d	0.088120	0.027778	0.832280
C	1_2	8d	0.911880	0.083333	0.167720
C	1_3	8d	0.088120	0.138889	0.832280
C	1_4	4c	0.088120	0.250000	0.832280
C	1_5	8d	0.088120	0.694444	0.832280
N	1	8d	0.127540	0.042530	0.720180
N	1_2	8d	0.872460	0.098086	0.279820
N	1_3	8d	0.627540	0.013026	0.779820
N	1_4	8d	0.127540	0.153641	0.720180
N	1_5	8d	0.127540	0.264752	0.720180
N	1_6	8d	0.127540	0.375863	0.720180
N	1_7	8d	0.127540	0.709197	0.720180
N	1_8	8d	0.127540	0.820308	0.720180
N	1_9	8d	0.127540	0.931419	0.720180

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
8d	(x,y,z)	S1	(0.992400,0.027778,0.114730)	S3	(0.999600,0.027760,0.113900)
8d	(x,y,z)	S1_2	(0.007600,0.083333,0.885270)	S4	(0.028000,0.083290,0.877200)
8d	(x,y,z)	S1_3	(0.992400,0.138889,0.114730)	S2	(0.021700,0.138970,0.102800)
4c	(x,1/4,z)	S1_4	(0.992400,0.250000,0.114730)	S1	(0.025300,0.250000,0.101600)
8d	(x,y,z)	S1_5	(0.992400,0.694444,0.114730)	S5	(0.957400,0.694330,0.125300)
8d	(x,y,z)	C1	(0.088120,0.027778,0.832280)	C3	(0.093900,0.027440,0.825800)
8d	(x,y,z)	C1_2	(0.911880,0.083333,0.167720)	C4	(0.917200,0.083560,0.152000)
8d	(x,y,z)	C1_3	(0.088120,0.138889,0.832280)	C2	(0.098500,0.138900,0.807900)
4c	(x,1/4,z)	C1_4	(0.088120,0.250000,0.832280)	C1	(0.102400,0.250000,0.806000)
8d	(x,y,z)	C1_5	(0.088120,0.694444,0.832280)	C5	(0.076100,0.694570,0.856400)
8d	(x,y,z)	N1	(0.127540,0.042530,0.720180)	N4	(0.130200,0.042100,0.708800)
8d	(x,y,z)	N1_2	(0.872460,0.098086,0.279820)	N7	(0.872600,0.098380,0.255500)
8d	(x,y,z)	N1_3	(0.627540,0.013026,0.779820)	N5	(0.630600,0.012550,0.784100)
8d	(x,y,z)	N1_4	(0.127540,0.153641,0.720180)	N2	(0.129500,0.153430,0.690100)
8d	(x,y,z)	N1_5	(0.127540,0.264752,0.720180)	N1	(0.130500,0.264760,0.687900)
8d	(x,y,z)	N1_6	(0.127540,0.375863,0.720180)	N3	(0.127300,0.376160,0.691300)
8d	(x,y,z)	N1_7	(0.127540,0.709197,0.720180)	N9	(0.123600,0.709310,0.754500)
8d	(x,y,z)	N1_8	(0.127540,0.820308,0.720180)	N8	(0.122500,0.820340,0.749200)
8d	(x,y,z)	N1_9	(0.127540,0.931419,0.720180)	N6	(0.129300,0.931170,0.742200)

WP		**Atom**	**Atomic Displacements**			
			u_x	u_y	u_z	|u|
8d	(x,y,z)	S1	0.0072	-0.0000	-0.0008	0.0545

8d	(x,y,z)	S1_2	0.0204	-0.0000	-0.0081	0.1602
8d	(x,y,z)	S1_3	0.0293	0.0001	-0.0119	0.2306
4c	(x,1/4,z)	S1_4	0.0329	0.0000	-0.0131	0.2584
8d	(x,y,z)	S1_5	-0.0350	-0.0001	0.0106	0.2705
8d	(x,y,z)	C1	0.0058	-0.0003	-0.0065	0.0619
8d	(x,y,z)	C1_2	0.0053	0.0002	-0.0157	0.0964
8d	(x,y,z)	C1_3	0.0104	0.0000	-0.0244	0.1546
4c	(x,1/4,z)	C1_4	0.0143	0.0000	-0.0263	0.1796
8d	(x,y,z)	C1_5	-0.0120	0.0001	0.0241	0.1603
8d	(x,y,z)	N1	0.0027	-0.0004	-0.0114	0.0733
8d	(x,y,z)	N1_2	0.0001	0.0003	-0.0243	0.1349
8d	(x,y,z)	N1_3	0.0031	-0.0005	0.0043	0.0492
8d	(x,y,z)	N1_4	0.0020	-0.0002	-0.0301	0.1659
8d	(x,y,z)	N1_5	0.0030	0.0000	-0.0323	0.1779
8d	(x,y,z)	N1_6	-0.0002	0.0003	-0.0289	0.1595
8d	(x,y,z)	N1_7	-0.0039	0.0001	0.0343	0.1902
8d	(x,y,z)	N1_8	-0.0050	0.0000	0.0290	0.1632
8d	(x,y,z)	N1_9	0.0018	-0.0002	0.0220	0.1226

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.2705 Å
Total distortion amplitude: 1.9093 Å

Symmetry Modes Summary

Atoms	WP	Modes
N1	8*d*	GM1+(3) **DT4(6) DT1(6)** DT4(6) **DT1(6)**
C1 S1	4*c*	GM1+(2) **DT4(3) DT1(3)** DT4(3) **DT1(3)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Pnma (62)	7	0.0799
(0,1/9,0)	DT4	(a,-5.671a)	Pnma (62)	12	1.8919
(0,2/9,0)	DT1	(a,0.364a)	Pnma (62)	12	0.1267
(0,1/3,0)	DT4	(a,-1.732a)	Pnma (62)	12	0.1872

(0,4/9,0)	DT1	(a,0.839a)	Pnma (62)	12	0.0899

Global distortion: 1.9091 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep GM1+

GM1+ Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.000000	0.030486
S1_2	0.000000	0.000000	-0.030486
S1_3	0.000000	0.000000	0.030486
S1_4	0.000000	0.000000	0.030486
S1_5	0.000000	0.000000	0.030486

GM1+ Mode S1 2

Atom	δx	δy	δz
S1	0.022090	-0.000000	-0.000000
S1_2	-0.022090	0.000000	0.000000
S1_3	0.022090	-0.000000	-0.000000
S1_4	0.022090	-0.000000	-0.000000
S1_5	0.022090	-0.000000	-0.000000

GM1+ Mode C1 1

Atom	δx	δy	δz
C1	0.000000	0.000000	0.030486
C1_2	0.000000	0.000000	-0.030486
C1_3	0.000000	0.000000	0.030486
C1_4	0.000000	0.000000	0.030486
C1_5	0.000000	0.000000	0.030486

GM1+ Mode C1 2

Atom	δx	δy	δz
C1	0.022090	-0.000000	-0.000000
C1_2	-0.022090	0.000000	0.000000
C1_3	0.022090	-0.000000	-0.000000

C1_4	0.022090	-0.000000	-0.000000
C1_5	0.022090	-0.000000	-0.000000

GM1+ Mode N1 1

Atom	δx	δy	δz
N1	0.000000	0.000000	0.021557
N1_2	0.000000	0.000000	-0.021557
N1_3	0.000000	0.000000	-0.021557
N1_4	0.000000	0.000000	0.021557
N1_5	0.000000	0.000000	0.021557
N1_6	0.000000	0.000000	0.021557
N1_7	0.000000	0.000000	0.021557
N1_8	0.000000	0.000000	0.021557
N1_9	0.000000	0.000000	0.021557

GM1+ Mode N1 2

Atom	δx	δy	δz
N1	0.000000	0.001533	-0.000000
N1_2	0.000000	0.001533	-0.000000
N1_3	0.000000	-0.001533	0.000000
N1_4	0.000000	0.001533	-0.000000
N1_5	0.000000	0.001533	-0.000000
N1_6	0.000000	0.001533	-0.000000
N1_7	0.000000	0.001533	-0.000000
N1_8	0.000000	0.001533	-0.000000
N1_9	0.000000	0.001533	-0.000000

GM1+ Mode N1 3

Atom	δx	δy	δz
N1	0.015620	-0.000000	-0.000000
N1_2	-0.015620	0.000000	0.000000
N1_3	0.015620	-0.000000	-0.000000
N1_4	0.015620	-0.000000	-0.000000
N1_5	0.015620	-0.000000	-0.000000
N1_6	0.015620	-0.000000	-0.000000
N1_7	0.015620	-0.000000	-0.000000

N1_8	0.015620	-0.000000	-0.000000
N1_9	0.015620	-0.000000	-0.000000

Irrep DT4

DT4 Mode S1 1

Atom	δx	δy	δz
S1	0.000000	-0.003020	0.000000
S1_2	0.000000	0.002655	-0.000000
S1_3	0.000000	-0.001972	0.000000
S1_4	0.000000	0.000000	0.000000
S1_5	0.000000	0.001048	-0.000000

DT4 Mode S1 2

Atom	δx	δy	δz
S1	0.000000	0.000000	0.007501
S1_2	0.000000	0.000000	0.021554
S1_3	0.000000	0.000000	0.033020
S1_4	0.000000	0.000000	0.043108
S1_5	0.000000	0.000000	-0.040521

DT4 Mode S1 3

Atom	δx	δy	δz
S1	0.005435	-0.000000	-0.000000
S1_2	0.015618	-0.000000	-0.000000
S1_3	0.023926	-0.000000	-0.000000
S1_4	0.031235	-0.000000	-0.000000
S1_5	-0.029361	0.000000	0.000000

DT4 Mode C1 1

Atom	δx	δy	δz
C1	0.005435	-0.000000	-0.000000
C1_2	0.015618	-0.000000	-0.000000
C1_3	0.023926	-0.000000	-0.000000
C1_4	0.031235	-0.000000	-0.000000
C1_5	-0.029361	0.000000	0.000000

DT4 Mode C1 2

Atom	δx	δy	δz
C1	0.000000	-0.003020	0.000000
C1_2	0.000000	0.002655	-0.000000
C1_3	0.000000	-0.001972	0.000000
C1_4	0.000000	0.000000	0.000000
C1_5	0.000000	0.001048	-0.000000

DT4 Mode C1 3

Atom	δx	δy	δz
C1	0.000000	0.000000	0.007501
C1_2	0.000000	0.000000	0.021554
C1_3	0.000000	0.000000	0.033020
C1_4	0.000000	0.000000	0.043108
C1_5	0.000000	0.000000	-0.040521

DT4 Mode N1 1

Atom	δx	δy	δz
N1	-0.021756	0.000000	0.000000
N1_2	-0.019124	0.000000	0.000000
N1_3	0.021756	-0.000000	-0.000000
N1_4	-0.014207	0.000000	0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	0.014207	-0.000000	-0.000000
N1_7	0.007549	-0.000000	-0.000000
N1_8	-0.007549	0.000000	0.000000
N1_9	-0.019124	0.000000	0.000000

DT4 Mode N1 2

Atom	δx	δy	δz
N1	0.000000	-0.002136	0.000000
N1_2	0.000000	0.001877	-0.000000
N1_3	0.000000	-0.002136	0.000000
N1_4	0.000000	-0.001395	0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	0.001395	-0.000000
N1_7	0.000000	0.000741	-0.000000

N1_8	0.000000	-0.000741	0.000000
N1_9	0.000000	-0.001877	0.000000

DT4 Mode N1 3

Atom	δx	δy	δz
N1	0.000000	0.000000	-0.030026
N1_2	0.000000	0.000000	-0.026393
N1_3	0.000000	0.000000	-0.030026
N1_4	0.000000	0.000000	-0.019607
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	0.000000	0.019607
N1_7	0.000000	0.000000	0.010419
N1_8	0.000000	0.000000	-0.010419
N1_9	0.000000	0.000000	-0.026393

DT4 Mode N1 4

Atom	δx	δy	δz
N1	0.000000	0.000000	0.005304
N1_2	0.000000	0.000000	0.015241
N1_3	0.000000	0.000000	-0.005304
N1_4	0.000000	0.000000	0.023349
N1_5	0.000000	0.000000	0.030482
N1_6	0.000000	0.000000	0.023349
N1_7	0.000000	0.000000	-0.028653
N1_8	0.000000	0.000000	-0.028653
N1_9	0.000000	0.000000	-0.015241

DT4 Mode N1 5

Atom	δx	δy	δz
N1	0.000000	0.000377	-0.000000
N1_2	0.000000	-0.001084	0.000000
N1_3	0.000000	-0.000377	0.000000
N1_4	0.000000	0.001661	-0.000000
N1_5	0.000000	0.002168	-0.000000
N1_6	0.000000	0.001661	-0.000000
N1_7	0.000000	-0.002038	0.000000

N1_8	0.000000	-0.002038	0.000000
N1_9	0.000000	-0.001084	0.000000

DT4 Mode N1 6

Atom	δx	δy	δz
N1	0.003843	-0.000000	-0.000000
N1_2	0.011043	-0.000000	-0.000000
N1_3	0.003843	-0.000000	-0.000000
N1_4	0.016918	-0.000000	-0.000000
N1_5	0.022087	-0.000000	-0.000000
N1_6	0.016918	-0.000000	-0.000000
N1_7	-0.020761	0.000000	0.000000
N1_8	-0.020761	0.000000	0.000000
N1_9	-0.011043	0.000000	0.000000

Irrep DT1

DT1 Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.000000	0.040521
S1_2	0.000000	0.000000	-0.021554
S1_3	0.000000	0.000000	-0.007501
S1_4	0.000000	0.000000	-0.043108
S1_5	0.000000	0.000000	-0.033020

DT1 Mode S1 2

Atom	δx	δy	δz
S1	0.000000	0.001048	-0.000000
S1_2	0.000000	0.002655	-0.000000
S1_3	0.000000	0.003020	-0.000000
S1_4	0.000000	0.000000	0.000000
S1_5	0.000000	0.001972	-0.000000

DT1 Mode S1 3

Atom	δx	δy	δz
S1	0.029361	-0.000000	-0.000000
S1_2	-0.015618	0.000000	0.000000

S1_3	-0.005435	0.000000	0.000000
S1_4	-0.031235	0.000000	0.000000
S1_5	-0.023926	0.000000	0.000000

DT1 Mode C1 1

Atom	δx	δy	δz
C1	0.000000	0.001048	-0.000000
C1_2	0.000000	0.002655	-0.000000
C1_3	0.000000	0.003020	-0.000000
C1_4	0.000000	0.000000	0.000000
C1_5	0.000000	0.001972	-0.000000

DT1 Mode C1 2

Atom	δx	δy	δz
C1	0.000000	0.000000	0.040521
C1_2	0.000000	0.000000	-0.021554
C1_3	0.000000	0.000000	-0.007501
C1_4	0.000000	0.000000	-0.043108
C1_5	0.000000	0.000000	-0.033020

DT1 Mode C1 3

Atom	δx	δy	δz
C1	0.029361	-0.000000	-0.000000
C1_2	-0.015618	0.000000	0.000000
C1_3	-0.005435	0.000000	0.000000
C1_4	-0.031235	0.000000	0.000000
C1_5	-0.023926	0.000000	0.000000

DT1 Mode N1 1

Atom	δx	δy	δz
N1	0.000000	0.000000	0.028653
N1_2	0.000000	0.000000	-0.015241
N1_3	0.000000	0.000000	-0.028653
N1_4	0.000000	0.000000	-0.005304
N1_5	0.000000	0.000000	-0.030482
N1_6	0.000000	0.000000	-0.005304
N1_7	0.000000	0.000000	-0.023349

N1_8	0.000000	0.000000	-0.023349
N1_9	0.000000	0.000000	0.015241

DT1 Mode N1 2

Atom	δx	δy	δz
N1	0.000000	0.000000	0.010419
N1_2	0.000000	0.000000	-0.026393
N1_3	0.000000	0.000000	0.010419
N1_4	0.000000	0.000000	0.030026
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	0.000000	-0.030026
N1_7	0.000000	0.000000	0.019607
N1_8	0.000000	0.000000	-0.019607
N1_9	0.000000	0.000000	-0.026393

DT1 Mode N1 3

Atom	δx	δy	δz
N1	0.000000	0.002038	-0.000000
N1_2	0.000000	0.001084	-0.000000
N1_3	0.000000	-0.002038	0.000000
N1_4	0.000000	-0.000377	0.000000
N1_5	0.000000	-0.002168	0.000000
N1_6	0.000000	-0.000377	0.000000
N1_7	0.000000	-0.001661	0.000000
N1_8	0.000000	-0.001661	0.000000
N1_9	0.000000	0.001084	-0.000000

DT1 Mode N1 4

Atom	δx	δy	δz
N1	0.000000	0.000741	-0.000000
N1_2	0.000000	0.001877	-0.000000
N1_3	0.000000	0.000741	-0.000000
N1_4	0.000000	0.002136	-0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	-0.002136	0.000000
N1_7	0.000000	0.001395	-0.000000

N1_8	0.000000	-0.001395	0.000000
N1_9	0.000000	-0.001877	0.000000

DT1 Mode N1 5

Atom	δx	δy	δz
N1	0.020761	-0.000000	-0.000000
N1_2	-0.011043	0.000000	0.000000
N1_3	0.020761	-0.000000	-0.000000
N1_4	-0.003843	0.000000	0.000000
N1_5	-0.022087	0.000000	0.000000
N1_6	-0.003843	0.000000	0.000000
N1_7	-0.016918	0.000000	0.000000
N1_8	-0.016918	0.000000	0.000000
N1_9	0.011043	-0.000000	-0.000000

DT1 Mode N1 6

Atom	δx	δy	δz
N1	0.007549	-0.000000	-0.000000
N1_2	-0.019124	0.000000	0.000000
N1_3	-0.007549	0.000000	0.000000
N1_4	0.021756	-0.000000	-0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	-0.021756	0.000000	0.000000
N1_7	0.014207	-0.000000	-0.000000
N1_8	-0.014207	0.000000	0.000000
N1_9	-0.019124	0.000000	0.000000

Irrep DT4

DT4 Mode S1 1

Atom	δx	δy	δz
S1	0.000000	-0.002656	0.000000
S1_2	0.000000	0.000000	0.000000
S1_3	0.000000	0.002656	-0.000000
S1_4	0.000000	0.000000	0.000000
S1_5	0.000000	-0.002656	0.000000

DT4 Mode S1 2

Atom	δx	δy	δz
S1	0.000000	0.000000	0.021557
S1_2	0.000000	0.000000	0.043114
S1_3	0.000000	0.000000	0.021557
S1_4	0.000000	0.000000	-0.043114
S1_5	0.000000	0.000000	0.021557

DT4 Mode S1 3

Atom	δx	δy	δz
S1	0.015620	-0.000000	-0.000000
S1_2	0.031240	-0.000000	-0.000000
S1_3	0.015620	-0.000000	-0.000000
S1_4	-0.031240	0.000000	0.000000
S1_5	0.015620	-0.000000	-0.000000

DT4 Mode C1 1

Atom	δx	δy	δz
C1	0.015620	-0.000000	-0.000000
C1_2	0.031240	-0.000000	-0.000000
C1_3	0.015620	-0.000000	-0.000000
C1_4	-0.031240	0.000000	0.000000
C1_5	0.015620	-0.000000	-0.000000

DT4 Mode C1 2

Atom	δx	δy	δz
C1	0.000000	0.000000	0.021557
C1_2	0.000000	0.000000	0.043114
C1_3	0.000000	0.000000	0.021557
C1_4	0.000000	0.000000	-0.043114
C1_5	0.000000	0.000000	0.021557

DT4 Mode C1 3

Atom	δx	δy	δz
C1	0.000000	-0.002656	0.000000
C1_2	0.000000	0.000000	0.000000
C1_3	0.000000	0.002656	-0.000000

C1_4	0.000000	0.000000	0.000000
C1_5	0.000000	-0.002656	0.000000

DT4 Mode N1 1

Atom	δx	δy	δz
N1	-0.019130	0.000000	0.000000
N1_2	0.000000	0.000000	0.000000
N1_3	0.019130	-0.000000	-0.000000
N1_4	0.019130	-0.000000	-0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	-0.019130	0.000000	0.000000
N1_7	-0.019130	0.000000	0.000000
N1_8	0.019130	-0.000000	-0.000000
N1_9	0.000000	0.000000	0.000000

DT4 Mode N1 2

Atom	δx	δy	δz
N1	0.000000	-0.001878	0.000000
N1_2	0.000000	0.000000	0.000000
N1_3	0.000000	-0.001878	0.000000
N1_4	0.000000	0.001878	-0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	-0.001878	0.000000
N1_7	0.000000	-0.001878	0.000000
N1_8	0.000000	0.001878	-0.000000
N1_9	0.000000	0.000000	0.000000

DT4 Mode N1 3

Atom	δx	δy	δz
N1	0.000000	0.000000	-0.026402
N1_2	0.000000	0.000000	0.000000
N1_3	0.000000	0.000000	-0.026402
N1_4	0.000000	0.000000	0.026402
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	0.000000	-0.026402
N1_7	0.000000	0.000000	-0.026402

N1_8	0.000000	0.000000	0.026402
N1_9	0.000000	0.000000	0.000000

DT4 Mode N1 4

Atom	δx	δy	δz
N1	0.000000	0.000000	0.015243
N1_2	0.000000	0.000000	0.030486
N1_3	0.000000	0.000000	-0.015243
N1_4	0.000000	0.000000	0.015243
N1_5	0.000000	0.000000	-0.030486
N1_6	0.000000	0.000000	0.015243
N1_7	0.000000	0.000000	0.015243
N1_8	0.000000	0.000000	0.015243
N1_9	0.000000	0.000000	-0.030486

DT4 Mode N1 5

Atom	δx	δy	δz
N1	0.000000	0.001084	-0.000000
N1_2	0.000000	-0.002168	0.000000
N1_3	0.000000	-0.001084	0.000000
N1_4	0.000000	0.001084	-0.000000
N1_5	0.000000	-0.002168	0.000000
N1_6	0.000000	0.001084	-0.000000
N1_7	0.000000	0.001084	-0.000000
N1_8	0.000000	0.001084	-0.000000
N1_9	0.000000	-0.002168	0.000000

DT4 Mode N1 6

Atom	δx	δy	δz
N1	0.011045	-0.000000	-0.000000
N1_2	0.022090	-0.000000	-0.000000
N1_3	0.011045	-0.000000	-0.000000
N1_4	0.011045	-0.000000	-0.000000
N1_5	-0.022090	0.000000	0.000000
N1_6	0.011045	-0.000000	-0.000000
N1_7	0.011045	-0.000000	-0.000000

N1_8	0.011045	-0.000000	-0.000000
N1_9	-0.022090	0.000000	0.000000

Irrep DT1

DT1 Mode S1 1

Atom	δx	δy	δz
S1	0.000000	0.000000	0.033020
S1_2	0.000000	0.000000	0.021554
S1_3	0.000000	0.000000	-0.040521
S1_4	0.000000	0.000000	0.043108
S1_5	0.000000	0.000000	0.007501

DT1 Mode S1 2

Atom	δx	δy	δz
S1	0.000000	0.001972	-0.000000
S1_2	0.000000	0.002655	-0.000000
S1_3	0.000000	-0.001048	0.000000
S1_4	0.000000	0.000000	0.000000
S1_5	0.000000	-0.003020	0.000000

DT1 Mode S1 3

Atom	δx	δy	δz
S1	0.023926	-0.000000	-0.000000
S1_2	0.015618	-0.000000	-0.000000
S1_3	-0.029361	0.000000	0.000000
S1_4	0.031235	-0.000000	-0.000000
S1_5	0.005435	-0.000000	-0.000000

DT1 Mode C1 1

Atom	δx	δy	δz
C1	0.023926	-0.000000	-0.000000
C1_2	0.015618	-0.000000	-0.000000
C1_3	-0.029361	0.000000	0.000000
C1_4	0.031235	-0.000000	-0.000000
C1_5	0.005435	-0.000000	-0.000000

DT1 Mode C1 2

Atom	δx	δy	δz
C1	0.000000	0.001972	-0.000000
C1_2	0.000000	0.002655	-0.000000
C1_3	0.000000	-0.001048	0.000000
C1_4	0.000000	0.000000	0.000000
C1_5	0.000000	-0.003020	0.000000

DT1 Mode C1 3

Atom	δx	δy	δz
C1	0.000000	0.000000	0.033020
C1_2	0.000000	0.000000	0.021554
C1_3	0.000000	0.000000	-0.040521
C1_4	0.000000	0.000000	0.043108
C1_5	0.000000	0.000000	0.007501

DT1 Mode N1 1

Atom	δx	δy	δz
N1	0.000000	0.000000	0.023349
N1_2	0.000000	0.000000	0.015241
N1_3	0.000000	0.000000	-0.023349
N1_4	0.000000	0.000000	-0.028653
N1_5	0.000000	0.000000	0.030482
N1_6	0.000000	0.000000	-0.028653
N1_7	0.000000	0.000000	0.005304
N1_8	0.000000	0.000000	0.005304
N1_9	0.000000	0.000000	-0.015241

DT1 Mode N1 2

Atom	δx	δy	δz
N1	0.000000	0.000000	0.019607
N1_2	0.000000	0.000000	-0.026393
N1_3	0.000000	0.000000	0.019607
N1_4	0.000000	0.000000	-0.010419
N1_5	0.000000	0.000000	-0.000000
N1_6	0.000000	0.000000	0.010419
N1_7	0.000000	0.000000	-0.030026

N1_8	0.000000	0.000000	0.030026
N1_9	0.000000	0.000000	-0.026393

DT1 Mode N1 3

Atom	δx	δy	δz
N1	0.000000	0.001661	-0.000000
N1_2	0.000000	-0.001084	0.000000
N1_3	0.000000	-0.001661	0.000000
N1_4	0.000000	-0.002038	0.000000
N1_5	0.000000	0.002168	-0.000000
N1_6	0.000000	-0.002038	0.000000
N1_7	0.000000	0.000377	-0.000000
N1_8	0.000000	0.000377	-0.000000
N1_9	0.000000	-0.001084	0.000000

DT1 Mode N1 4

Atom	δx	δy	δz
N1	0.000000	0.001395	-0.000000
N1_2	0.000000	0.001877	-0.000000
N1_3	0.000000	0.001395	-0.000000
N1_4	0.000000	-0.000741	0.000000
N1_5	0.000000	0.000000	0.000000
N1_6	0.000000	0.000741	-0.000000
N1_7	0.000000	-0.002136	0.000000
N1_8	0.000000	0.002136	-0.000000
N1_9	0.000000	-0.001877	0.000000

DT1 Mode N1 5

Atom	δx	δy	δz
N1	0.016918	-0.000000	-0.000000
N1_2	0.011043	-0.000000	-0.000000
N1_3	0.016918	-0.000000	-0.000000
N1_4	-0.020761	0.000000	0.000000
N1_5	0.022087	-0.000000	-0.000000
N1_6	-0.020761	0.000000	0.000000
N1_7	0.003843	-0.000000	-0.000000

N1_8	0.003843	-0.000000	-0.000000
N1_9	-0.011043	0.000000	0.000000

DT1 Mode N1 6

Atom	δx	δy	δz
N1	0.014207	-0.000000	-0.000000
N1_2	-0.019124	0.000000	0.000000
N1_3	-0.014207	0.000000	0.000000
N1_4	-0.007549	0.000000	0.000000
N1_5	-0.000000	0.000000	0.000000
N1_6	0.007549	-0.000000	-0.000000
N1_7	-0.021756	0.000000	0.000000
N1_8	0.021756	-0.000000	-0.000000
N1_9	-0.019124	0.000000	0.000000

K-vector: GM = (0,0,0)

Irrep: GM1+

Direction: (a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      1      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{GM1+}= 0.0799 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

S1 1	S1 2	C1 1	C1 2	N1 1	N1 2	N1 3
-0.0625	-0.3083	-0.3793	0.7500	0.1792	0.2991	0.2705

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
S1	-0.0068	0.0000	-0.0019

S1_2	0.0068	-0.0000	0.0019
S1_3	-0.0068	0.0000	-0.0019
S1_4	-0.0068	0.0000	-0.0019
S1_5	-0.0068	0.0000	-0.0019
C1	0.0166	-0.0000	-0.0116
C1_2	-0.0166	0.0000	0.0116
C1_3	0.0166	-0.0000	-0.0116
C1_4	0.0166	-0.0000	-0.0116
C1_5	0.0166	-0.0000	-0.0116
N1	0.0042	0.0005	0.0039
N1_2	-0.0042	0.0005	-0.0039
N1_3	0.0042	-0.0005	-0.0039
N1_4	0.0042	0.0005	0.0039
N1_5	0.0042	0.0005	0.0039
N1_6	0.0042	0.0005	0.0039
N1_7	0.0042	0.0005	0.0039
N1_8	0.0042	0.0005	0.0039
N1_9	0.0042	0.0005	0.0039

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: DT = (0,1/9,0)

Irrep: DT4

Direction: (a,-5.671a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      9      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{DT4}= 1.8919 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

S1 1	S1 2	S1 3	C1 1	C1 2	C1 3	N1 1	N1 2	N1 3	N1 4	N1 5	N1 6

-0.0085	-0.1625	0.6259	0.2260	0.0433	-0.3458	-0.0122	0.0930	0.0446	-0.6275	-0.0042	0.0686

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
S1	0.0034	0.0000	-0.0012
S1_2	0.0098	-0.0000	-0.0035
S1_3	0.0150	0.0000	-0.0054
S1_4	0.0196	-0.0000	-0.0070
S1_5	-0.0184	-0.0000	0.0066
C1	0.0012	-0.0001	-0.0026
C1_2	0.0035	0.0001	-0.0075
C1_3	0.0054	-0.0001	-0.0114
C1_4	0.0071	-0.0000	-0.0149
C1_5	-0.0066	0.0000	0.0140
N1	0.0005	-0.0002	-0.0047
N1_2	0.0010	0.0002	-0.0107
N1_3	-0.0000	-0.0002	0.0020
N1_4	0.0013	-0.0001	-0.0155
N1_5	0.0015	-0.0000	-0.0191
N1_6	0.0010	0.0001	-0.0138
N1_7	-0.0015	0.0001	0.0184
N1_8	-0.0013	-0.0001	0.0175
N1_9	-0.0005	-0.0002	0.0084

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: DT-2 = (0,2/9,0)

Irrep: DT1

Direction: (a,0.364a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      9      0 ] [      0]
```

```
[      0      0      1 ] [       0]
```

The amplitude of this distortion is:
A_{DT1}= 0.1267 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

S1 1	S1 2	S1 3	C1 1	C1 2	C1 3	N1 1	N1 2	N1 3	N1 4	N1 5	N1 6
0.3092	-0.0423	0.2055	0.1978	0.0549	0.3408	0.1421	0.1031	-0.0553	-0.2329	0.7788	0.0868

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
S1	0.0060	-0.0000	0.0125
S1_2	-0.0032	-0.0001	-0.0067
S1_3	-0.0011	-0.0001	-0.0023
S1_4	-0.0064	0.0000	-0.0133
S1_5	-0.0049	-0.0001	-0.0102
C1	0.0100	0.0002	0.0022
C1_2	-0.0053	0.0005	-0.0012
C1_3	-0.0019	0.0006	-0.0004
C1_4	-0.0106	0.0000	-0.0024
C1_5	-0.0082	0.0004	-0.0018
N1	0.0168	-0.0003	0.0051
N1_2	-0.0103	-0.0005	-0.0049
N1_3	0.0155	-0.0001	-0.0030
N1_4	-0.0011	-0.0005	0.0023
N1_5	-0.0172	0.0001	-0.0043
N1_6	-0.0049	0.0005	-0.0039
N1_7	-0.0119	-0.0002	-0.0013
N1_8	-0.0144	0.0004	-0.0053
N1_9	0.0069	0.0004	-0.0006

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: DT-3 = (0,1/3,0)

Irrep: DT4

Direction: (a,-1.732a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      3      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{DT4}= 0.1872 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

S1 1	S1 2	S1 3	C1 1	C1 2	C1 3	N1 1	N1 2	N1 3	N1 4	N1 5	N1 6
0.1428	-0.1432	0.3572	0.0190	-0.3277	0.1496	0.0698	0.1503	0.0202	-0.7672	0.0468	-0.2875

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
S1	0.0056	-0.0004	-0.0031
S1_2	0.0112	-0.0000	-0.0062
S1_3	0.0056	0.0004	-0.0031
S1_4	-0.0112	0.0000	0.0062
S1_5	0.0056	-0.0004	-0.0031
C1	0.0003	-0.0004	-0.0071
C1_2	0.0006	-0.0000	-0.0141
C1_3	0.0003	0.0004	-0.0071
C1_4	-0.0006	0.0000	0.0141
C1_5	0.0003	-0.0004	-0.0071
N1	-0.0045	-0.0002	-0.0122
N1_2	-0.0064	-0.0001	-0.0234
N1_3	-0.0018	-0.0003	0.0112
N1_4	-0.0018	0.0003	-0.0112
N1_5	0.0064	-0.0001	0.0234
N1_6	-0.0045	-0.0002	-0.0122
N1_7	-0.0045	-0.0002	-0.0122
N1_8	-0.0018	0.0003	-0.0112
N1_9	0.0064	-0.0001	0.0234

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: DT-4 = (0,4/9,0)

Irrep: DT1

Direction: (a,0.839a)

Isotropy Subgroup: 62 Pnma D2h-16

Transformation matrix:

```
[      1      0      0 ] [      0]
[      0      9      0 ] [      0]
[      0      0      1 ] [      0]
```

The amplitude of this distortion is:
A_{DT1}= 0.0899 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

S1 1	S1 2	S1 3	C1 1	C1 2	C1 3	N1 1	N1 2	N1 3	N1 4	N1 5	N1 6
0.2084	0.0577	-0.2321	0.3764	-0.2398	0.1319	-0.0812	-0.5988	-0.0398	-0.0214	0.3751	-0.4182

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
S1	-0.0056	0.0001	0.0069
S1_2	-0.0036	0.0002	0.0045
S1_3	0.0068	-0.0001	-0.0084
S1_4	-0.0073	0.0000	0.0090
S1_5	-0.0013	-0.0002	0.0016
C1	0.0090	-0.0005	0.0044
C1_2	0.0059	-0.0006	0.0028
C1_3	-0.0111	0.0003	-0.0053
C1_4	0.0118	-0.0000	0.0057
C1_5	0.0020	0.0007	0.0010
N1	0.0004	-0.0001	-0.0136
N1_2	0.0121	0.0000	0.0146
N1_3	0.0123	0.0000	-0.0098

N1_4	-0.0046	0.0001	0.0086
N1_5	0.0083	-0.0001	-0.0025
N1_6	-0.0109	0.0001	-0.0039
N1_7	0.0105	0.0000	0.0175
N1_8	-0.0077	-0.0001	-0.0184
N1_9	0.0039	0.0001	0.0170

Virtual structure with only this symmetry component of the distortion frozen.

Ga-Phase Ga-II

Ref: O. Degtyareva,* M. I. McMahon, D. R. Allan, and R. J. Nelmes Phys. Rev. Lett. 93, 205502 (2004)

Symmetry mode analysis

High symmetry structure

```
70
5.976 8.576 2.75062 90 90 90
1
Ga      1       8a      0.125000        0.125000        0.125000
```

Low symmetry structure

```
20
5.976 8.576 35.758 90 90 90
14
Ga      1       4b      0.500000        0.180200        0.250000
Ga      2       8c      0.695600        0.468400        0.271600
Ga      3       8c      0.580400        0.785800        0.286100
Ga      4       8c      0.277200        0.562200        0.308100
Ga      5       8c      -0.034100       0.780900        0.329200
Ga      6       8c      0.848200        0.456700        0.343000
Ga      7       8c      0.563200        0.691900        0.366600
Ga      8       8c      0.232400        0.483800        0.385100
Ga      9       8c      0.612900        0.291400        0.400300
Ga      10      8c      0.827600        0.566000        0.425000
Ga      11      8c      -0.003000       0.261300        0.443500
Ga      12      4a      0.246000        0.000000        0.500000
Ga      13      8c      0.105200        0.309000        0.517000
Ga      14      8c      0.357400        0.551800        0.540900
```

Transformation matrix

```
[      1      0      0  ] [    -1/8]
[      0      1      0  ] [     1/8]
[      0      0     13  ] [    -3/8]
```

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
020
5.976000 8.576000 35.758060 90.000000 90.000000 90.000000
14
Ga      1       8c      0.250000        0.000000        0.038462
Ga      1_2     8c      0.750000        0.000000        0.076923
Ga      1_3     8c      0.000000        0.750000        0.019231
Ga      1_4     8c      0.500000        0.750000        0.057692
Ga      1_5     8c      0.500000        0.250000        0.096154
Ga      1_6     8c      0.250000        0.000000        0.115385
```

```
Ga      1_7     8c      0.250000        0.000000        0.192308
Ga      1_8     8c      0.250000        0.000000        0.269231
Ga      1_9     8c      0.250000        0.000000        0.346154
Ga      1_10    4a      0.250000        0.000000        0.500000
Ga      1_11    8c      0.500000        0.750000        0.134615
Ga      1_12    8c      0.500000        0.250000        0.173077
Ga      1_13    8c      0.500000        0.750000        0.211538
Ga      1_14    4b      0.500000        0.250000        0.250000
```

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Reference Struc.**	**Atom**	**Low Sym Struc.**
8c	(x,y,z)	Ga1	(0.250000,0.000000,0.038462)	Ga14	(0.142600,0.948200,0.040900)
8c	(x,y,z)	Ga1_2	(0.750000,0.000000,0.076923)	Ga10	(0.672400,0.066000,0.075000)
8c	(x,y,z)	Ga1_3	(0.000000,0.750000,0.019231)	Ga13	(0.894800,0.691000,0.017000)
8c	(x,y,z)	Ga1_4	(0.500000,0.750000,0.057692)	Ga11	(0.503000,0.761300,0.056500)
8c	(x,y,z)	Ga1_5	(0.500000,0.250000,0.096154)	Ga9	(0.387100,0.291400,0.099700)
8c	(x,y,z)	Ga1_6	(0.250000,0.000000,0.115385)	Ga8	(0.267600,0.983800,0.114900)
8c	(x,y,z)	Ga1_7	(0.250000,0.000000,0.192308)	Ga4	(0.222800,0.062200,0.191900)
8c	(x,y,z)	Ga1_8	(0.250000,0.000000,0.269231)	Ga2	(0.195600,0.968400,0.271600)
8c	(x,y,z)	Ga1_9	(0.250000,0.000000,0.346154)	Ga6	(0.348200,0.956700,0.343000)
4a	(x,0,0)	Ga1_10	(0.250000,0.000000,0.500000)	Ga12	(0.246000,0.000000,0.500000)
8c	(x,y,z)	Ga1_11	(0.500000,0.750000,0.134615)	Ga7	(0.436800,0.691900,0.133400)
8c	(x,y,z)	Ga1_12	(0.500000,0.250000,0.173077)	Ga5	(0.534100,0.280900,0.170800)
8c	(x,y,z)	Ga1_13	(0.500000,0.750000,0.211538)	Ga3	(0.419600,0.785800,0.213900)
4b	(0,y,1/4)	Ga1_14	(0.500000,0.250000,0.250000)	Ga1	(0.500000,0.180200,0.250000)

WP		**Atom**	**Atomic Displacements**			
			u_x	u_y	u_z	|u|
8c	(x,y,z)	Ga1	-0.1074	-0.0518	0.0024	0.7854
8c	(x,y,z)	Ga1_2	-0.0776	0.0660	-0.0019	0.7350
8c	(x,y,z)	Ga1_3	-0.1052	-0.0590	-0.0022	0.8109
8c	(x,y,z)	Ga1_4	0.0030	0.0113	-0.0012	0.1074
8c	(x,y,z)	Ga1_5	-0.1129	0.0414	0.0035	0.7729
8c	(x,y,z)	Ga1_6	0.0176	-0.0162	-0.0005	0.1751

8c	(x,y,z)	Ga1_7	-0.0272	0.0622	-0.0004	0.5578
8c	(x,y,z)	Ga1_8	-0.0544	-0.0316	0.0024	0.4316
8c	(x,y,z)	Ga1_9	0.0982	-0.0433	-0.0032	0.7036
4a	(x,0,0)	Ga1_10	-0.0040	0.0000	0.0000	0.0239
8c	(x,y,z)	Ga1_11	-0.0632	-0.0581	-0.0012	0.6267
8c	(x,y,z)	Ga1_12	0.0341	0.0309	-0.0023	0.3441
8c	(x,y,z)	Ga1_13	-0.0804	0.0358	0.0024	0.5764
4b	(0,y,1/4)	Ga1_14	0.0000	-0.0698	0.0000	0.5986

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.8109 Å
Total distortion amplitude: 4.2282 Å

Symmetry Modes Summary

Atoms	WP	Modes
Ga1	8*a*	**LD3(2) LD4(2)** LD1(1) LD2(1) **LD3(2) LD4(2)** LD1(1) LD2(1) **LD3(2) LD4(2)** LD1(1) LD2(1) **LD3(2) LD4(2)** LD1(1) LD2(1) **LD3(2) LD4(2)** LD1(1) LD2(1) Z2(2)

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,1/13)	LD3	(a,0.690a)	C222_1 (20)	2	0.1104
(0,0,1/13)	LD4	(a,0.690a)	C222_1 (20)	2	2.1401
(0,0,2/13)	LD1	(a,2.637a)	F222 (22)	1	0.0334
(0,0,2/13)	LD2	(a,2.637a)	Fddd (70)	1	0.0329
(0,0,3/13)	LD3	(a,-4.057a)	C222_1 (20)	2	0.0589
(0,0,3/13)	LD4	(a,-4.057a)	C222_1 (20)	2	0.0537
(0,0,4/13)	LD1	(a,-0.886a)	Fddd (70)	1	0.0032
(0,0,4/13)	LD2	(a,-0.886a)	F222 (22)	1	0.0309
(0,0,5/13)	LD3	(a,-0.121a)	C222_1 (20)	2	0.0452
(0,0,5/13)	LD4	(a,-0.121a)	C222_1 (20)	2	0.1106
(0,0,6/13)	LD1	(a,0.525a)	F222 (22)	1	0.0597

(0,0,6/13)	LD2	(a,0.525a)	Fddd (70)	1	0.0060
(0,0,7/13)	LD3	(a,1.905a)	C222_1 (20)	2	0.1556
(0,0,7/13)	LD4	(a,1.905a)	C222_1 (20)	2	0.1086
(0,0,8/13)	LD1	(a,-8.236a)	Fddd (70)	1	0.0271
(0,0,8/13)	LD2	(a,-8.236a)	F222 (22)	1	0.5297
(0,0,9/13)	LD3	(a,-1.129a)	C222_1 (20)	2	3.5933
(0,0,9/13)	LD4	(a,-1.129a)	C222_1 (20)	2	0.0537
(0,0,10/13)	LD1	(a,-0.246a)	F222 (22)	1	0.0222
(0,0,10/13)	LD2	(a,-0.246a)	Fddd (70)	1	0.0028
(0,0,11/13)	LD3	(a,0.379a)	C222_1 (20)	2	0.1247
(0,0,11/13)	LD4	(a,0.379a)	C222_1 (20)	2	0.0456
(0,0,12/13)	LD1	(a,1.449a)	Fddd (70)	1	0.0429
(0,0,12/13)	LD2	(a,1.449a)	F222 (22)	1	0.0132
(0,0,1)	Z2	(a,a)	C222_1 (20)	2	0.0722

Global distortion: 4.2281 Å

Normalized Symmetry modes

The modes are normalized to the reference structure unit cell and are given as relative displacements in this cell.

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.031863	-0.000000	-0.000000
Ga1_2	0.029041	-0.000000	-0.000000
Ga1_3	-0.032585	0.000000	0.000000
Ga1_4	-0.030682	0.000000	0.000000
Ga1_5	-0.027007	0.000000	0.000000
Ga1_6	0.024578	-0.000000	-0.000000
Ga1_7	0.011649	-0.000000	-0.000000
Ga1_8	-0.003971	0.000000	0.000000
Ga1_9	-0.018639	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000

Ga1_11	-0.021756	0.000000	0.000000
Ga1_12	-0.015259	0.000000	0.000000
Ga1_13	-0.007843	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	-0.005465	0.000000
Ga1_2	0.000000	-0.010633	0.000000
Ga1_3	0.000000	-0.002767	0.000000
Ga1_4	0.000000	-0.008118	0.000000
Ga1_5	0.000000	-0.012988	0.000000
Ga1_6	0.000000	-0.015160	0.000000
Ga1_7	0.000000	-0.021380	0.000000
Ga1_8	0.000000	-0.022706	0.000000
Ga1_9	0.000000	-0.018819	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.017127	0.000000
Ga1_12	0.000000	-0.020237	0.000000
Ga1_13	0.000000	-0.022203	0.000000
Ga1_14	0.000000	-0.022866	0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.031863	-0.000000	-0.000000
Ga1_2	0.029041	-0.000000	-0.000000
Ga1_3	0.032585	-0.000000	-0.000000
Ga1_4	0.030682	-0.000000	-0.000000
Ga1_5	0.027007	-0.000000	-0.000000
Ga1_6	0.024578	-0.000000	-0.000000
Ga1_7	0.011649	-0.000000	-0.000000

Ga1_8	-0.003971	0.000000	0.000000
Ga1_9	-0.018639	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000
Ga1_11	0.021756	-0.000000	-0.000000
Ga1_12	0.015259	-0.000000	-0.000000
Ga1_13	0.007843	-0.000000	-0.000000
Ga1_14	0.000000	0.000000	0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	-0.005465	0.000000
Ga1_2	0.000000	-0.010633	0.000000
Ga1_3	0.000000	0.002767	-0.000000
Ga1_4	0.000000	0.008118	-0.000000
Ga1_5	0.000000	0.012988	-0.000000
Ga1_6	0.000000	-0.015160	0.000000
Ga1_7	0.000000	-0.021380	0.000000
Ga1_8	0.000000	-0.022706	0.000000
Ga1_9	0.000000	-0.018819	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.017127	-0.000000
Ga1_12	0.000000	0.020237	-0.000000
Ga1_13	0.000000	0.022203	-0.000000
Ga1_14	0.000000	0.022866	-0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	-0.002548
Ga1_2	0.000000	0.000000	-0.004513
Ga1_3	0.000000	0.000000	-0.001312
Ga1_4	0.000000	0.000000	-0.003637

Ga1_5	0.000000	0.000000	-0.005129
Ga1_6	0.000000	0.000000	-0.005445
Ga1_7	0.000000	0.000000	-0.003637
Ga1_8	0.000000	0.000000	0.001312
Ga1_9	0.000000	0.000000	0.005129
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.005445
Ga1_12	0.000000	0.000000	-0.004513
Ga1_13	0.000000	0.000000	-0.002548
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	-0.002548
Ga1_2	0.000000	0.000000	-0.004513
Ga1_3	0.000000	0.000000	0.001312
Ga1_4	0.000000	0.000000	0.003637
Ga1_5	0.000000	0.000000	0.005129
Ga1_6	0.000000	0.000000	-0.005445
Ga1_7	0.000000	0.000000	-0.003637
Ga1_8	0.000000	0.000000	0.001312
Ga1_9	0.000000	0.000000	0.005129
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.005445
Ga1_12	0.000000	0.000000	0.004513
Ga1_13	0.000000	0.000000	0.002548
Ga1_14	0.000000	0.000000	0.000000

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.015160	-0.000000
Ga1_2	0.000000	0.022706	-0.000000
Ga1_3	0.000000	0.008118	-0.000000
Ga1_4	0.000000	0.020237	-0.000000
Ga1_5	0.000000	0.022203	-0.000000
Ga1_6	0.000000	0.018819	-0.000000
Ga1_7	0.000000	-0.010633	0.000000
Ga1_8	0.000000	-0.021380	0.000000
Ga1_9	0.000000	0.005465	-0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.012988	-0.000000
Ga1_12	0.000000	-0.002767	0.000000
Ga1_13	0.000000	-0.017127	0.000000
Ga1_14	0.000000	-0.022866	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	-0.024578	0.000000	0.000000
Ga1_2	-0.003971	0.000000	0.000000
Ga1_3	0.030682	-0.000000	-0.000000
Ga1_4	0.015259	-0.000000	-0.000000
Ga1_5	-0.007843	0.000000	0.000000
Ga1_6	0.018639	-0.000000	-0.000000
Ga1_7	0.029041	-0.000000	-0.000000
Ga1_8	-0.011649	0.000000	0.000000
Ga1_9	-0.031863	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	-0.027007	0.000000	0.000000
Ga1_12	-0.032585	0.000000	0.000000
Ga1_13	-0.021756	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.015160	-0.000000
Ga1_2	0.000000	0.022706	-0.000000
Ga1_3	0.000000	-0.008118	0.000000
Ga1_4	0.000000	-0.020237	0.000000
Ga1_5	0.000000	-0.022203	0.000000
Ga1_6	0.000000	0.018819	-0.000000
Ga1_7	0.000000	-0.010633	0.000000
Ga1_8	0.000000	-0.021380	0.000000
Ga1_9	0.000000	0.005465	-0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.012988	0.000000
Ga1_12	0.000000	0.002767	-0.000000
Ga1_13	0.000000	0.017127	-0.000000
Ga1_14	0.000000	0.022866	-0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	-0.024578	0.000000	0.000000
Ga1_2	-0.003971	0.000000	0.000000
Ga1_3	-0.030682	0.000000	0.000000
Ga1_4	-0.015259	0.000000	0.000000
Ga1_5	0.007843	-0.000000	-0.000000
Ga1_6	0.018639	-0.000000	-0.000000
Ga1_7	0.029041	-0.000000	-0.000000
Ga1_8	-0.011649	0.000000	0.000000
Ga1_9	-0.031863	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	0.027007	-0.000000	-0.000000
Ga1_12	0.032585	-0.000000	-0.000000
Ga1_13	0.021756	-0.000000	-0.000000

Ga1_14	0.000000	0.000000	0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.004513
Ga1_2	0.000000	0.000000	0.005129
Ga1_3	0.000000	0.000000	0.002548
Ga1_4	0.000000	0.000000	0.005445
Ga1_5	0.000000	0.000000	0.003637
Ga1_6	0.000000	0.000000	0.001312
Ga1_7	0.000000	0.000000	-0.005445
Ga1_8	0.000000	0.000000	0.002548
Ga1_9	0.000000	0.000000	0.003637
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.001312
Ga1_12	0.000000	0.000000	-0.005129
Ga1_13	0.000000	0.000000	-0.004513
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.004513
Ga1_2	0.000000	0.000000	0.005129
Ga1_3	0.000000	0.000000	-0.002548
Ga1_4	0.000000	0.000000	-0.005445
Ga1_5	0.000000	0.000000	-0.003637
Ga1_6	0.000000	0.000000	0.001312
Ga1_7	0.000000	0.000000	-0.005445
Ga1_8	0.000000	0.000000	0.002548

Ga1_9	0.000000	0.000000	0.003637
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.001312
Ga1_12	0.000000	0.000000	0.005129
Ga1_13	0.000000	0.000000	0.004513
Ga1_14	0.000000	0.000000	0.000000

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.011649	-0.000000	-0.000000
Ga1_2	-0.024578	0.000000	0.000000
Ga1_3	-0.027007	0.000000	0.000000
Ga1_4	0.007843	-0.000000	-0.000000
Ga1_5	0.032585	-0.000000	-0.000000
Ga1_6	-0.029041	0.000000	0.000000
Ga1_7	0.031863	-0.000000	-0.000000
Ga1_8	-0.018639	0.000000	0.000000
Ga1_9	-0.003971	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000
Ga1_11	0.015259	-0.000000	-0.000000
Ga1_12	-0.021756	0.000000	0.000000
Ga1_13	-0.030682	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.021380	-0.000000
Ga1_2	0.000000	0.015160	-0.000000
Ga1_3	0.000000	0.012988	-0.000000
Ga1_4	0.000000	0.022203	-0.000000
Ga1_5	0.000000	0.002767	-0.000000

Ga1_6	0.000000	-0.010633	0.000000
Ga1_7	0.000000	-0.005465	0.000000
Ga1_8	0.000000	0.018819	-0.000000
Ga1_9	0.000000	-0.022706	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.020237	0.000000
Ga1_12	0.000000	-0.017127	0.000000
Ga1_13	0.000000	0.008118	-0.000000
Ga1_14	0.000000	0.022866	-0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.011649	-0.000000	-0.000000
Ga1_2	-0.024578	0.000000	0.000000
Ga1_3	0.027007	-0.000000	-0.000000
Ga1_4	-0.007843	0.000000	0.000000
Ga1_5	-0.032585	0.000000	0.000000
Ga1_6	-0.029041	0.000000	0.000000
Ga1_7	0.031863	-0.000000	-0.000000
Ga1_8	-0.018639	0.000000	0.000000
Ga1_9	-0.003971	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000
Ga1_11	-0.015259	0.000000	0.000000
Ga1_12	0.021756	-0.000000	-0.000000
Ga1_13	0.030682	-0.000000	-0.000000
Ga1_14	0.000000	0.000000	0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.021380	-0.000000
Ga1_2	0.000000	0.015160	-0.000000

Ga1_3	0.000000	-0.012988	0.000000
Ga1_4	0.000000	-0.022203	0.000000
Ga1_5	0.000000	-0.002767	0.000000
Ga1_6	0.000000	-0.010633	0.000000
Ga1_7	0.000000	-0.005465	0.000000
Ga1_8	0.000000	0.018819	-0.000000
Ga1_9	0.000000	-0.022706	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.020237	-0.000000
Ga1_12	0.000000	0.017127	-0.000000
Ga1_13	0.000000	-0.008118	0.000000
Ga1_14	0.000000	-0.022866	0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.005445
Ga1_2	0.000000	0.000000	0.001312
Ga1_3	0.000000	0.000000	0.003637
Ga1_4	0.000000	0.000000	0.004513
Ga1_5	0.000000	0.000000	-0.002548
Ga1_6	0.000000	0.000000	-0.005129
Ga1_7	0.000000	0.000000	0.004513
Ga1_8	0.000000	0.000000	-0.003637
Ga1_9	0.000000	0.000000	0.002548
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.005129
Ga1_12	0.000000	0.000000	0.001312
Ga1_13	0.000000	0.000000	0.005445
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.005445
Ga1_2	0.000000	0.000000	0.001312
Ga1_3	0.000000	0.000000	-0.003637
Ga1_4	0.000000	0.000000	-0.004513
Ga1_5	0.000000	0.000000	0.002548
Ga1_6	0.000000	0.000000	-0.005129
Ga1_7	0.000000	0.000000	0.004513
Ga1_8	0.000000	0.000000	-0.003637
Ga1_9	0.000000	0.000000	0.002548
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.005129
Ga1_12	0.000000	0.000000	-0.001312
Ga1_13	0.000000	0.000000	-0.005445
Ga1_14	0.000000	0.000000	0.000000

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.022706	-0.000000
Ga1_2	0.000000	-0.005465	0.000000
Ga1_3	0.000000	0.017127	-0.000000
Ga1_4	0.000000	0.012988	-0.000000
Ga1_5	0.000000	-0.020237	0.000000
Ga1_6	0.000000	-0.021380	0.000000
Ga1_7	0.000000	0.018819	-0.000000
Ga1_8	0.000000	-0.015160	0.000000
Ga1_9	0.000000	0.010633	-0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.008118	0.000000
Ga1_12	0.000000	0.022203	-0.000000

Ga1_13	0.000000	0.002767	-0.000000
Ga1_14	0.000000	-0.022866	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	-0.003971	0.000000	0.000000
Ga1_2	-0.031863	0.000000	0.000000
Ga1_3	-0.021756	0.000000	0.000000
Ga1_4	0.027007	-0.000000	-0.000000
Ga1_5	0.015259	-0.000000	-0.000000
Ga1_6	0.011649	-0.000000	-0.000000
Ga1_7	-0.018639	0.000000	0.000000
Ga1_8	0.024578	-0.000000	-0.000000
Ga1_9	-0.029041	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000
Ga1_11	-0.030682	0.000000	0.000000
Ga1_12	-0.007843	0.000000	0.000000
Ga1_13	0.032585	-0.000000	-0.000000
Ga1_14	0.000000	0.000000	0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.022706	-0.000000
Ga1_2	0.000000	-0.005465	0.000000
Ga1_3	0.000000	-0.017127	0.000000
Ga1_4	0.000000	-0.012988	0.000000
Ga1_5	0.000000	0.020237	-0.000000
Ga1_6	0.000000	-0.021380	0.000000
Ga1_7	0.000000	0.018819	-0.000000
Ga1_8	0.000000	-0.015160	0.000000
Ga1_9	0.000000	0.010633	-0.000000

Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.008118	-0.000000
Ga1_12	0.000000	-0.022203	0.000000
Ga1_13	0.000000	-0.002767	0.000000
Ga1_14	0.000000	0.022866	-0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	-0.003971	0.000000	0.000000
Ga1_2	-0.031863	0.000000	0.000000
Ga1_3	0.021756	-0.000000	-0.000000
Ga1_4	-0.027007	0.000000	0.000000
Ga1_5	-0.015259	0.000000	0.000000
Ga1_6	0.011649	-0.000000	-0.000000
Ga1_7	-0.018639	0.000000	0.000000
Ga1_8	0.024578	-0.000000	-0.000000
Ga1_9	-0.029041	0.000000	0.000000
Ga1_10	-0.032815	0.000000	0.000000
Ga1_11	0.030682	-0.000000	-0.000000
Ga1_12	0.007843	-0.000000	-0.000000
Ga1_13	-0.032585	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	-0.005129
Ga1_2	0.000000	0.000000	0.003637
Ga1_3	0.000000	0.000000	-0.004513
Ga1_4	0.000000	0.000000	-0.001312
Ga1_5	0.000000	0.000000	0.005445
Ga1_6	0.000000	0.000000	0.002548

Ga1_7	0.000000	0.000000	0.001312
Ga1_8	0.000000	0.000000	-0.004513
Ga1_9	0.000000	0.000000	0.005445
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.002548
Ga1_12	0.000000	0.000000	-0.003637
Ga1_13	0.000000	0.000000	0.005129
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	-0.005129
Ga1_2	0.000000	0.000000	0.003637
Ga1_3	0.000000	0.000000	0.004513
Ga1_4	0.000000	0.000000	0.001312
Ga1_5	0.000000	0.000000	-0.005445
Ga1_6	0.000000	0.000000	0.002548
Ga1_7	0.000000	0.000000	0.001312
Ga1_8	0.000000	0.000000	-0.004513
Ga1_9	0.000000	0.000000	0.005445
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.002548
Ga1_12	0.000000	0.000000	0.003637
Ga1_13	0.000000	0.000000	-0.005129
Ga1_14	0.000000	0.000000	0.000000

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.018639	-0.000000	-0.000000

Ga1_2	0.011649	-0.000000	-0.000000
Ga1_3	0.015259	-0.000000	-0.000000
Ga1_4	-0.032585	0.000000	0.000000
Ga1_5	0.021756	-0.000000	-0.000000
Ga1_6	-0.031863	0.000000	0.000000
Ga1_7	0.003971	-0.000000	-0.000000
Ga1_8	0.029041	-0.000000	-0.000000
Ga1_9	-0.024578	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	0.007843	-0.000000	-0.000000
Ga1_12	-0.030682	0.000000	0.000000
Ga1_13	0.027007	-0.000000	-0.000000
Ga1_14	0.000000	0.000000	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.018819	-0.000000
Ga1_2	0.000000	-0.021380	0.000000
Ga1_3	0.000000	0.020237	-0.000000
Ga1_4	0.000000	-0.002767	0.000000
Ga1_5	0.000000	-0.017127	0.000000
Ga1_6	0.000000	0.005465	-0.000000
Ga1_7	0.000000	-0.022706	0.000000
Ga1_8	0.000000	0.010633	-0.000000
Ga1_9	0.000000	0.015160	-0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.022203	-0.000000
Ga1_12	0.000000	-0.008118	0.000000
Ga1_13	0.000000	-0.012988	0.000000
Ga1_14	0.000000	0.022866	-0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.018639	-0.000000	-0.000000
Ga1_2	0.011649	-0.000000	-0.000000
Ga1_3	-0.015259	0.000000	0.000000
Ga1_4	0.032585	-0.000000	-0.000000
Ga1_5	-0.021756	0.000000	0.000000
Ga1_6	-0.031863	0.000000	0.000000
Ga1_7	0.003971	-0.000000	-0.000000
Ga1_8	0.029041	-0.000000	-0.000000
Ga1_9	-0.024578	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	-0.007843	0.000000	0.000000
Ga1_12	0.030682	-0.000000	-0.000000
Ga1_13	-0.027007	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.018819	-0.000000
Ga1_2	0.000000	-0.021380	0.000000
Ga1_3	0.000000	-0.020237	0.000000
Ga1_4	0.000000	0.002767	-0.000000
Ga1_5	0.000000	0.017127	-0.000000
Ga1_6	0.000000	0.005465	-0.000000
Ga1_7	0.000000	-0.022706	0.000000
Ga1_8	0.000000	0.010633	-0.000000
Ga1_9	0.000000	0.015160	-0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.022203	0.000000
Ga1_12	0.000000	0.008118	-0.000000
Ga1_13	0.000000	0.012988	-0.000000
Ga1_14	0.000000	-0.022866	0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.003637
Ga1_2	0.000000	0.000000	-0.005445
Ga1_3	0.000000	0.000000	0.005129
Ga1_4	0.000000	0.000000	-0.002548
Ga1_5	0.000000	0.000000	-0.001312
Ga1_6	0.000000	0.000000	0.004513
Ga1_7	0.000000	0.000000	-0.002548
Ga1_8	0.000000	0.000000	-0.005129
Ga1_9	0.000000	0.000000	0.001312
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.004513
Ga1_12	0.000000	0.000000	-0.005445
Ga1_13	0.000000	0.000000	0.003637
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.003637
Ga1_2	0.000000	0.000000	-0.005445
Ga1_3	0.000000	0.000000	-0.005129
Ga1_4	0.000000	0.000000	0.002548
Ga1_5	0.000000	0.000000	0.001312
Ga1_6	0.000000	0.000000	0.004513
Ga1_7	0.000000	0.000000	-0.002548
Ga1_8	0.000000	0.000000	-0.005129
Ga1_9	0.000000	0.000000	0.001312

Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.004513
Ga1_12	0.000000	0.000000	0.005445
Ga1_13	0.000000	0.000000	-0.003637
Ga1_14	0.000000	0.000000	0.000000

Irrep LD3

LD3 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.029041	-0.000000	-0.000000
Ga1_2	-0.018639	0.000000	0.000000
Ga1_3	0.007843	-0.000000	-0.000000
Ga1_4	-0.021756	0.000000	0.000000
Ga1_5	0.030682	-0.000000	-0.000000
Ga1_6	0.003971	-0.000000	-0.000000
Ga1_7	-0.024578	0.000000	0.000000
Ga1_8	-0.031863	0.000000	0.000000
Ga1_9	-0.011649	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	-0.032585	0.000000	0.000000
Ga1_12	0.027007	-0.000000	-0.000000
Ga1_13	-0.015259	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

LD3 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.010633	-0.000000
Ga1_2	0.000000	-0.018819	0.000000
Ga1_3	0.000000	0.022203	-0.000000
Ga1_4	0.000000	-0.017127	0.000000
Ga1_5	0.000000	0.008118	-0.000000
Ga1_6	0.000000	0.022706	-0.000000

Ga1_7	0.000000	0.015160	-0.000000
Ga1_8	0.000000	-0.005465	0.000000
Ga1_9	0.000000	-0.021380	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.002767	-0.000000
Ga1_12	0.000000	-0.012988	0.000000
Ga1_13	0.000000	0.020237	-0.000000
Ga1_14	0.000000	-0.022866	0.000000

Irrep LD4

LD4 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.029041	-0.000000	-0.000000
Ga1_2	-0.018639	0.000000	0.000000
Ga1_3	-0.007843	0.000000	0.000000
Ga1_4	0.021756	-0.000000	-0.000000
Ga1_5	-0.030682	0.000000	0.000000
Ga1_6	0.003971	-0.000000	-0.000000
Ga1_7	-0.024578	0.000000	0.000000
Ga1_8	-0.031863	0.000000	0.000000
Ga1_9	-0.011649	0.000000	0.000000
Ga1_10	0.032815	-0.000000	-0.000000
Ga1_11	0.032585	-0.000000	-0.000000
Ga1_12	-0.027007	0.000000	0.000000
Ga1_13	0.015259	-0.000000	-0.000000
Ga1_14	0.000000	0.000000	0.000000

LD4 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.010633	-0.000000
Ga1_2	0.000000	-0.018819	0.000000
Ga1_3	0.000000	-0.022203	0.000000

Ga1_4	0.000000	0.017127	-0.000000
Ga1_5	0.000000	-0.008118	0.000000
Ga1_6	0.000000	0.022706	-0.000000
Ga1_7	0.000000	0.015160	-0.000000
Ga1_8	0.000000	-0.005465	0.000000
Ga1_9	0.000000	-0.021380	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	-0.002767	0.000000
Ga1_12	0.000000	0.012988	-0.000000
Ga1_13	0.000000	-0.020237	0.000000
Ga1_14	0.000000	0.022866	-0.000000

Irrep LD1

LD1 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.001312
Ga1_2	0.000000	0.000000	-0.002548
Ga1_3	0.000000	0.000000	0.005445
Ga1_4	0.000000	0.000000	-0.005129
Ga1_5	0.000000	0.000000	0.004513
Ga1_6	0.000000	0.000000	0.003637
Ga1_7	0.000000	0.000000	0.005129
Ga1_8	0.000000	0.000000	0.005445
Ga1_9	0.000000	0.000000	0.004513
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	-0.003637
Ga1_12	0.000000	0.000000	0.002548
Ga1_13	0.000000	0.000000	-0.001312
Ga1_14	0.000000	0.000000	0.000000

Irrep LD2

LD2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.001312
Ga1_2	0.000000	0.000000	-0.002548
Ga1_3	0.000000	0.000000	-0.005445
Ga1_4	0.000000	0.000000	0.005129
Ga1_5	0.000000	0.000000	-0.004513
Ga1_6	0.000000	0.000000	0.003637
Ga1_7	0.000000	0.000000	0.005129
Ga1_8	0.000000	0.000000	0.005445
Ga1_9	0.000000	0.000000	0.004513
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.000000	0.003637
Ga1_12	0.000000	0.000000	-0.002548
Ga1_13	0.000000	0.000000	0.001312
Ga1_14	0.000000	0.000000	0.000000

Irrep Z2

Z2 Mode Ga1 1

Atom	δx	δy	δz
Ga1	0.032817	-0.000000	-0.000000
Ga1_2	-0.032817	0.000000	0.000000
Ga1_3	0.000000	0.000000	0.000000
Ga1_4	0.000000	0.000000	0.000000
Ga1_5	0.000000	0.000000	0.000000
Ga1_6	0.032817	-0.000000	-0.000000
Ga1_7	0.032817	-0.000000	-0.000000
Ga1_8	0.032817	-0.000000	-0.000000
Ga1_9	0.032817	-0.000000	-0.000000
Ga1_10	0.032817	-0.000000	-0.000000
Ga1_11	0.000000	0.000000	0.000000
Ga1_12	0.000000	0.000000	0.000000

Ga1_13	0.000000	0.000000	0.000000
Ga1_14	0.000000	0.000000	0.000000

Z2 Mode Ga1 2

Atom	δx	δy	δz
Ga1	0.000000	0.000000	0.000000
Ga1_2	0.000000	0.000000	0.000000
Ga1_3	0.000000	-0.022868	0.000000
Ga1_4	0.000000	0.022868	-0.000000
Ga1_5	0.000000	-0.022868	0.000000
Ga1_6	0.000000	0.000000	0.000000
Ga1_7	0.000000	0.000000	0.000000
Ga1_8	0.000000	0.000000	0.000000
Ga1_9	0.000000	0.000000	0.000000
Ga1_10	0.000000	0.000000	0.000000
Ga1_11	0.000000	0.022868	-0.000000
Ga1_12	0.000000	-0.022868	0.000000
Ga1_13	0.000000	0.022868	-0.000000
Ga1_14	0.000000	-0.022868	0.000000

K-vector: LD = (0,0,1/13)

Irrep: LD3

Direction: (a,0.690a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 0.1104 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.9854	-0.1701

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0314	0.0009	-0.0000
Ga1_2	0.0286	0.0018	-0.0000
Ga1_3	-0.0321	0.0005	0.0000
Ga1_4	-0.0302	0.0014	0.0000
Ga1_5	-0.0266	0.0022	0.0000
Ga1_6	0.0242	0.0026	-0.0000
Ga1_7	0.0115	0.0036	-0.0000
Ga1_8	-0.0039	0.0039	-0.0000
Ga1_9	-0.0184	0.0032	0.0000
Ga1_10	-0.0323	0.0000	0.0000
Ga1_11	-0.0214	0.0029	0.0000
Ga1_12	-0.0150	0.0034	0.0000
Ga1_13	-0.0077	0.0038	0.0000
Ga1_14	0.0000	0.0039	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,0.690a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:

A_{LD4}= 2.1401 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.9999	0.0169

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	-0.0319	-0.0001	0.0000
Ga1_2	-0.0290	-0.0002	0.0000
Ga1_3	-0.0326	0.0000	0.0000
Ga1_4	-0.0307	0.0001	0.0000
Ga1_5	-0.0270	0.0002	0.0000
Ga1_6	-0.0246	-0.0003	0.0000
Ga1_7	-0.0116	-0.0004	0.0000
Ga1_8	0.0040	-0.0004	-0.0000
Ga1_9	0.0186	-0.0003	-0.0000
Ga1_10	0.0328	-0.0000	-0.0000
Ga1_11	-0.0218	0.0003	0.0000
Ga1_12	-0.0153	0.0003	0.0000
Ga1_13	-0.0078	0.0004	0.0000
Ga1_14	0.0000	0.0004	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-2 = (0,0,2/13)

Irrep: LD1

Direction: (a,2.637a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD1}= 0.0334 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0334

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0025
Ga1_2	0.0000	0.0000	0.0045
Ga1_3	0.0000	0.0000	0.0013
Ga1_4	0.0000	0.0000	0.0036
Ga1_5	0.0000	0.0000	0.0051
Ga1_6	0.0000	0.0000	0.0054
Ga1_7	0.0000	0.0000	0.0036
Ga1_8	0.0000	0.0000	-0.0013
Ga1_9	0.0000	0.0000	-0.0051
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	0.0054
Ga1_12	0.0000	0.0000	0.0045
Ga1_13	0.0000	0.0000	0.0025
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,2.637a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[      1      0      0 ] [     1/4]
[      0      0     -1 ] [     3/2]
[      0     13      0 ] [  -21/4]
```

The amplitude of this distortion is:
A_{LD2}= 0.0329 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0329

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0025
Ga1_2	0.0000	0.0000	0.0045
Ga1_3	0.0000	0.0000	-0.0013
Ga1_4	0.0000	0.0000	-0.0036
Ga1_5	0.0000	0.0000	-0.0051
Ga1_6	0.0000	0.0000	0.0054
Ga1_7	0.0000	0.0000	0.0036
Ga1_8	0.0000	0.0000	-0.0013
Ga1_9	0.0000	0.0000	-0.0051
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0054
Ga1_12	0.0000	0.0000	-0.0045
Ga1_13	0.0000	0.0000	-0.0025
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-3 = (0,0,3/13)

Irrep: LD3

Direction: (a,-4.057a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 0.0589 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.9979	-0.0644

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0016	0.0151	-0.0000
Ga1_2	0.0003	0.0227	-0.0000
Ga1_3	-0.0020	0.0081	-0.0000
Ga1_4	-0.0010	0.0202	-0.0000
Ga1_5	0.0005	0.0222	-0.0000
Ga1_6	-0.0012	0.0188	-0.0000
Ga1_7	-0.0019	-0.0106	0.0000
Ga1_8	0.0008	-0.0213	0.0000
Ga1_9	0.0021	0.0055	-0.0000
Ga1_10	-0.0021	0.0000	0.0000
Ga1_11	0.0017	0.0130	-0.0000
Ga1_12	0.0021	-0.0028	0.0000
Ga1_13	0.0014	-0.0171	0.0000
Ga1_14	0.0000	-0.0228	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,-4.057a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0  ] [    -1/8]
[      0      1      0  ] [     1/8]
[      0      0     13  ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD4}= 0.0537 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.9446	-0.3282

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0081	0.0143	-0.0000
Ga1_2	0.0013	0.0214	-0.0000
Ga1_3	0.0101	-0.0077	0.0000
Ga1_4	0.0050	-0.0191	0.0000
Ga1_5	-0.0026	-0.0210	0.0000
Ga1_6	-0.0061	0.0178	-0.0000
Ga1_7	-0.0095	-0.0100	0.0000
Ga1_8	0.0038	-0.0202	0.0000
Ga1_9	0.0105	0.0052	-0.0000
Ga1_10	-0.0108	0.0000	0.0000
Ga1_11	-0.0089	-0.0123	0.0000
Ga1_12	-0.0107	0.0026	0.0000
Ga1_13	-0.0071	0.0162	-0.0000
Ga1_14	0.0000	0.0216	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-4 = (0,0,4/13)

Irrep: LD1

Direction: (a,-0.886a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[     1      0      0 ] [    1/4]
[     0      0     -1 ] [    3/2]
[     0     13      0 ] [ -21/4]
```

The amplitude of this distortion is:
A_{LD1}= 0.0032 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
0.0032

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0045
Ga1_2	0.0000	0.0000	0.0051
Ga1_3	0.0000	0.0000	0.0025
Ga1_4	0.0000	0.0000	0.0054
Ga1_5	0.0000	0.0000	0.0036
Ga1_6	0.0000	0.0000	0.0013
Ga1_7	0.0000	0.0000	-0.0054
Ga1_8	0.0000	0.0000	0.0025
Ga1_9	0.0000	0.0000	0.0036
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0013
Ga1_12	0.0000	0.0000	-0.0051

Ga1_13	0.0000	0.0000	-0.0045
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,-0.886a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD2}= 0.0309 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0309

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	-0.0045
Ga1_2	0.0000	0.0000	-0.0051
Ga1_3	0.0000	0.0000	0.0025
Ga1_4	0.0000	0.0000	0.0054
Ga1_5	0.0000	0.0000	0.0036
Ga1_6	0.0000	0.0000	-0.0013
Ga1_7	0.0000	0.0000	0.0054
Ga1_8	0.0000	0.0000	-0.0025
Ga1_9	0.0000	0.0000	-0.0036
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0013

Ga1_12	0.0000	0.0000	-0.0051
Ga1_13	0.0000	0.0000	-0.0045
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-5 = (0,0,5/13)

Irrep: LD3

Direction: (a,-0.121a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 0.0452 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.2708	-0.9626

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	-0.0032	-0.0206	0.0000
Ga1_2	0.0067	-0.0146	0.0000
Ga1_3	0.0073	-0.0125	0.0000
Ga1_4	-0.0021	-0.0214	0.0000
Ga1_5	-0.0088	-0.0027	0.0000
Ga1_6	0.0079	0.0102	-0.0000
Ga1_7	-0.0086	0.0053	0.0000

Ga1_8	0.0050	-0.0181	0.0000
Ga1_9	0.0011	0.0219	-0.0000
Ga1_10	0.0089	-0.0000	-0.0000
Ga1_11	-0.0041	0.0195	-0.0000
Ga1_12	0.0059	0.0165	-0.0000
Ga1_13	0.0083	-0.0078	0.0000
Ga1_14	0.0000	-0.0220	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,-0.121a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD4}= 0.1106 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.0280	0.9996

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0003	0.0214	-0.0000
Ga1_2	-0.0007	0.0152	-0.0000
Ga1_3	0.0008	-0.0130	0.0000
Ga1_4	-0.0002	-0.0222	0.0000

Ga1_5	-0.0009	-0.0028	0.0000
Ga1_6	-0.0008	-0.0106	0.0000
Ga1_7	0.0009	-0.0055	0.0000
Ga1_8	-0.0005	0.0188	-0.0000
Ga1_9	-0.0001	-0.0227	0.0000
Ga1_10	-0.0009	0.0000	0.0000
Ga1_11	-0.0004	0.0202	-0.0000
Ga1_12	0.0006	0.0171	-0.0000
Ga1_13	0.0009	-0.0081	0.0000
Ga1_14	0.0000	-0.0229	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-6 = (0,0,6/13)

Irrep: LD1

Direction: (a,0.525a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD1}= 0.0597 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0597

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	-0.0054

Ga1_2	0.0000	0.0000	-0.0013
Ga1_3	0.0000	0.0000	-0.0036
Ga1_4	0.0000	0.0000	-0.0045
Ga1_5	0.0000	0.0000	0.0025
Ga1_6	0.0000	0.0000	0.0051
Ga1_7	0.0000	0.0000	-0.0045
Ga1_8	0.0000	0.0000	0.0036
Ga1_9	0.0000	0.0000	-0.0025
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	0.0051
Ga1_12	0.0000	0.0000	-0.0013
Ga1_13	0.0000	0.0000	-0.0054
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,0.525a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[      1      0      0 ] [     1/4]
[      0      0     -1 ] [     3/2]
[      0     13      0 ] [  -21/4]
```

The amplitude of this distortion is:
A_{LD2}= 0.0060 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
0.0060

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz

Ga1	0.0000	0.0000	0.0054
Ga1_2	0.0000	0.0000	0.0013
Ga1_3	0.0000	0.0000	-0.0036
Ga1_4	0.0000	0.0000	-0.0045
Ga1_5	0.0000	0.0000	0.0025
Ga1_6	0.0000	0.0000	-0.0051
Ga1_7	0.0000	0.0000	0.0045
Ga1_8	0.0000	0.0000	-0.0036
Ga1_9	0.0000	0.0000	0.0025
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	0.0051
Ga1_12	0.0000	0.0000	-0.0013
Ga1_13	0.0000	0.0000	-0.0054
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-7 = (0,0,7/13)

Irrep: LD3

Direction: (a,1.905a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0  ] [    -1/8]
[      0      1      0  ] [     1/8]
[      0      0     13  ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 0.1556 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.6653	-0.7466

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0030	0.0151	-0.0000
Ga1_2	0.0238	-0.0036	-0.0000
Ga1_3	0.0162	0.0114	-0.0000
Ga1_4	-0.0202	0.0086	0.0000
Ga1_5	-0.0114	-0.0135	0.0000
Ga1_6	-0.0087	-0.0142	0.0000
Ga1_7	0.0139	0.0125	-0.0000
Ga1_8	-0.0184	-0.0101	0.0000
Ga1_9	0.0217	0.0071	-0.0000
Ga1_10	0.0245	-0.0000	-0.0000
Ga1_11	0.0229	-0.0054	-0.0000
Ga1_12	0.0059	0.0148	-0.0000
Ga1_13	-0.0243	0.0018	0.0000
Ga1_14	0.0000	-0.0152	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,1.905a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD4}= 0.1086 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.9607	-0.2777

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0011	-0.0218	0.0000
Ga1_2	0.0088	0.0053	-0.0000
Ga1_3	-0.0060	0.0165	-0.0000
Ga1_4	0.0075	0.0125	-0.0000
Ga1_5	0.0042	-0.0194	0.0000
Ga1_6	-0.0032	0.0205	-0.0000
Ga1_7	0.0052	-0.0181	0.0000
Ga1_8	-0.0068	0.0146	-0.0000
Ga1_9	0.0081	-0.0102	0.0000
Ga1_10	0.0091	-0.0000	-0.0000
Ga1_11	-0.0085	-0.0078	0.0000
Ga1_12	-0.0022	0.0213	-0.0000
Ga1_13	0.0090	0.0027	-0.0000
Ga1_14	0.0000	-0.0220	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-8 = (0,0,8/13)

Irrep: LD1

Direction: (a,-8.236a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[      1      0      0 ] [     1/4]
[      0      0     -1 ] [     3/2]
[      0     13      0 ] [   -21/4]
```

The amplitude of this distortion is:
A_{LD1}= 0.0271 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
0.0271

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	-0.0051
Ga1_2	0.0000	0.0000	0.0036
Ga1_3	0.0000	0.0000	-0.0045
Ga1_4	0.0000	0.0000	-0.0013
Ga1_5	0.0000	0.0000	0.0054
Ga1_6	0.0000	0.0000	0.0025
Ga1_7	0.0000	0.0000	0.0013
Ga1_8	0.0000	0.0000	-0.0045
Ga1_9	0.0000	0.0000	0.0054
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0025
Ga1_12	0.0000	0.0000	-0.0036
Ga1_13	0.0000	0.0000	0.0051
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,-8.236a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD2}= 0.5297 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.5297

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0051
Ga1_2	0.0000	0.0000	-0.0036
Ga1_3	0.0000	0.0000	-0.0045
Ga1_4	0.0000	0.0000	-0.0013
Ga1_5	0.0000	0.0000	0.0054
Ga1_6	0.0000	0.0000	-0.0025
Ga1_7	0.0000	0.0000	-0.0013
Ga1_8	0.0000	0.0000	0.0045
Ga1_9	0.0000	0.0000	-0.0054
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0025
Ga1_12	0.0000	0.0000	-0.0036
Ga1_13	0.0000	0.0000	0.0051
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-9 = (0,0,9/13)

Irrep: LD3

Direction: (a,-1.129a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 3.5933 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.6164	-0.7874

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	-0.0115	-0.0148	0.0000
Ga1_2	-0.0072	0.0168	-0.0000
Ga1_3	-0.0094	-0.0159	0.0000
Ga1_4	0.0201	0.0022	-0.0000
Ga1_5	-0.0134	0.0135	-0.0000
Ga1_6	0.0196	-0.0043	-0.0000
Ga1_7	-0.0024	0.0179	-0.0000
Ga1_8	-0.0179	-0.0084	0.0000
Ga1_9	0.0152	-0.0119	0.0000
Ga1_10	-0.0202	0.0000	0.0000
Ga1_11	-0.0048	-0.0175	0.0000
Ga1_12	0.0189	0.0064	-0.0000
Ga1_13	-0.0166	0.0102	0.0000
Ga1_14	0.0000	-0.0180	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,-1.129a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD4}= 0.0537 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.6351	-0.7725

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0118	-0.0145	0.0000
Ga1_2	0.0074	0.0165	-0.0000
Ga1_3	-0.0097	0.0156	-0.0000
Ga1_4	0.0207	-0.0021	-0.0000
Ga1_5	-0.0138	-0.0132	0.0000
Ga1_6	-0.0202	-0.0042	0.0000
Ga1_7	0.0025	0.0175	-0.0000
Ga1_8	0.0184	-0.0082	-0.0000
Ga1_9	-0.0156	-0.0117	0.0000
Ga1_10	0.0208	-0.0000	-0.0000
Ga1_11	-0.0050	0.0172	-0.0000
Ga1_12	0.0195	-0.0063	-0.0000
Ga1_13	-0.0172	-0.0100	0.0000
Ga1_14	0.0000	0.0177	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-10 = (0,0,10/13)

Irrep: LD1

Direction: (a,-0.246a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD1}= 0.0222 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
0.0222

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0036
Ga1_2	0.0000	0.0000	-0.0054
Ga1_3	0.0000	0.0000	0.0051
Ga1_4	0.0000	0.0000	-0.0025
Ga1_5	0.0000	0.0000	-0.0013
Ga1_6	0.0000	0.0000	0.0045
Ga1_7	0.0000	0.0000	-0.0025
Ga1_8	0.0000	0.0000	-0.0051
Ga1_9	0.0000	0.0000	0.0013
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	0.0045
Ga1_12	0.0000	0.0000	-0.0054
Ga1_13	0.0000	0.0000	0.0036
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,-0.246a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[      1      0      0 ] [     1/4]
[      0      0     -1 ] [     3/2]
[      0     13      0 ] [  -21/4]
```

The amplitude of this distortion is:
A_{LD2}= 0.0028 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0028

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	-0.0036
Ga1_2	0.0000	0.0000	0.0054
Ga1_3	0.0000	0.0000	0.0051
Ga1_4	0.0000	0.0000	-0.0025
Ga1_5	0.0000	0.0000	-0.0013
Ga1_6	0.0000	0.0000	-0.0045
Ga1_7	0.0000	0.0000	0.0025
Ga1_8	0.0000	0.0000	0.0051
Ga1_9	0.0000	0.0000	-0.0013
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	0.0045
Ga1_12	0.0000	0.0000	-0.0054
Ga1_13	0.0000	0.0000	0.0036
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-11 = (0,0,11/13)

Irrep: LD3

Direction: (a,0.379a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0 ] [    -1/8]
[      0      1      0 ] [     1/8]
[      0      0     13 ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD3}= 0.1247 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.6386	-0.7695

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	-0.0185	-0.0082	0.0000
Ga1_2	0.0119	0.0145	-0.0000
Ga1_3	-0.0050	-0.0171	0.0000
Ga1_4	0.0139	0.0132	-0.0000
Ga1_5	-0.0196	-0.0062	0.0000
Ga1_6	-0.0025	-0.0175	0.0000
Ga1_7	0.0157	-0.0117	0.0000
Ga1_8	0.0203	0.0042	-0.0000
Ga1_9	0.0074	0.0165	-0.0000
Ga1_10	-0.0210	0.0000	0.0000

Ga1_11	0.0208	-0.0021	-0.0000
Ga1_12	-0.0172	0.0100	0.0000
Ga1_13	0.0097	-0.0156	0.0000
Ga1_14	0.0000	0.0176	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD4

Direction: (a,0.379a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[      1      0      0  ] [    -1/8]
[      0      1      0  ] [     1/8]
[      0      0     13  ] [    -3/8]
```

The amplitude of this distortion is:
A_{LD4}= 0.0456 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
-0.8244	0.5661

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	-0.0239	0.0060	0.0000
Ga1_2	0.0154	-0.0107	-0.0000
Ga1_3	0.0065	-0.0126	0.0000
Ga1_4	-0.0179	0.0097	0.0000
Ga1_5	0.0253	-0.0046	-0.0000
Ga1_6	-0.0033	0.0129	-0.0000
Ga1_7	0.0203	0.0086	-0.0000

Ga1_8	0.0263	-0.0031	-0.0000
Ga1_9	0.0096	-0.0121	0.0000
Ga1_10	-0.0271	0.0000	0.0000
Ga1_11	-0.0269	-0.0016	0.0000
Ga1_12	0.0223	0.0074	-0.0000
Ga1_13	-0.0126	-0.0115	0.0000
Ga1_14	0.0000	0.0129	-0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: LD-12 = (0,0,12/13)

Irrep: LD1

Direction: (a,1.449a)

Isotropy Subgroup: 70 Fddd D2h-24

Transformation matrix:

```
[      1      0      0  ] [     1/4]
[      0      0     -1  ] [     3/2]
[      0     13      0  ] [  -21/4]
```

The amplitude of this distortion is:
A_{LD1}= 0.0429 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
0.0429

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	0.0013
Ga1_2	0.0000	0.0000	-0.0025
Ga1_3	0.0000	0.0000	0.0054
Ga1_4	0.0000	0.0000	-0.0051

Ga1_5	0.0000	0.0000	0.0045
Ga1_6	0.0000	0.0000	0.0036
Ga1_7	0.0000	0.0000	0.0051
Ga1_8	0.0000	0.0000	0.0054
Ga1_9	0.0000	0.0000	0.0045
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0036
Ga1_12	0.0000	0.0000	0.0025
Ga1_13	0.0000	0.0000	-0.0013
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

Irrep: LD2

Direction: (a,1.449a)

Isotropy Subgroup: 22 F222 D2-7

Transformation matrix:

```
[      1      0      0 ] [    11/8]
[      0      0     -1 ] [     3/8]
[      0     13      0 ] [    75/8]
```

The amplitude of this distortion is:
A_{LD2}= 0.0132 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

Ga1 1
-0.0132

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0000	0.0000	-0.0013
Ga1_2	0.0000	0.0000	0.0025
Ga1_3	0.0000	0.0000	0.0054

Ga1_4	0.0000	0.0000	-0.0051
Ga1_5	0.0000	0.0000	0.0045
Ga1_6	0.0000	0.0000	-0.0036
Ga1_7	0.0000	0.0000	-0.0051
Ga1_8	0.0000	0.0000	-0.0054
Ga1_9	0.0000	0.0000	-0.0045
Ga1_10	0.0000	0.0000	0.0000
Ga1_11	0.0000	0.0000	-0.0036
Ga1_12	0.0000	0.0000	0.0025
Ga1_13	0.0000	0.0000	-0.0013
Ga1_14	0.0000	0.0000	0.0000

Virtual structure with only this symmetry component of the distortion frozen.

K-vector: Z = (0,0,1)

Irrep: Z2

Direction: (a,a)

Isotropy Subgroup: 20 C222_1 D2-5

Transformation matrix:

```
[     1     0     0 ] [    3/8]
[     0     1     0 ] [    1/8]
[     0     0     1 ] [    1/8]
```

The amplitude of this distortion is:
A_{Z2}= 0.0722 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized) atomic symmetry modes)

Ga1 1	Ga1 2
0.1559	0.9878

NOTE: A second number next to the label counts the different symmetry modes that may happen for that orbit.

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Ga1	0.0051	-0.0000	-0.0000
Ga1_2	-0.0051	0.0000	0.0000
Ga1_3	0.0000	-0.0226	0.0000
Ga1_4	0.0000	0.0226	-0.0000
Ga1_5	0.0000	-0.0226	0.0000
Ga1_6	0.0051	-0.0000	-0.0000
Ga1_7	0.0051	-0.0000	-0.0000
Ga1_8	0.0051	-0.0000	-0.0000
Ga1_9	0.0051	-0.0000	-0.0000
Ga1_10	0.0051	-0.0000	-0.0000
Ga1_11	0.0000	0.0226	-0.0000
Ga1_12	0.0000	-0.0226	0.0000
Ga1_13	0.0000	0.0226	-0.0000
Ga1_14	0.0000	-0.0226	0.0000

Virtual structure with only this symmetry component of the distortion frozen.