Monoclinic phase of the system $PbZr_{1-x}Ti_xO_3$

Problem: Consider the perovskite-like ferroelectric system $PbZr_{1-x}Ti_xO_3$ (PZT). Recent measurements have revealed a monoclinic phase between the previously established tetragonal and rhombohedral regions. According to the structure analysis, the monoclinic structure can be considered as a providing a 'bridge' between the rhombohedral and tetragonal regions of the morphotropic phase boundary (see Fig.3).

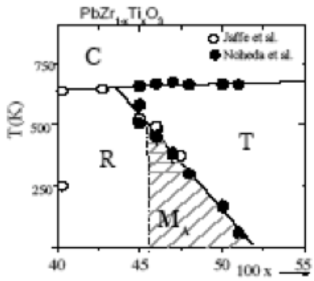


Fig.3. Phase diagram of PZT in the vicinity of its morphotropic phase boundary. C, R, and T represent cubic, rhombohedral and tetragonal regions. The diagonally-shaded M_A area represents the stability region of monoclinic phase. (D.E. Cox et al. Condensed Matter, cond-mat/0102457, 2001.)

Using the structure data for the tetragonal and rhombohedral phase, show that the space-group Cm as a symmetry group for the monoclinic phase (no cell multiplication) satisfies the symmetry conditions for a maximal-symmetry transition path, namely:

1. Common subgroup: the space group Cm (no cell multiplication) is a common subgroup of the symmetry groups of the tetragonal phase ($P4mm$) and that of the rhombohedral phase ($R3m$);
2. Compatibility of the occupied Wyckoff orbits in the common subgroup;
3. Maximal-symmetry transition path.

Structure 1

Space Group *P4mm* (99) with Z=1 (formula units per conventional unit cell)

Cell parameters

a	4.0460	**b**	4.0460	**c**	4.1394
α	90	**β**	90	**γ**	90

Atoms

ATOM	WP	Rep.	Orbit
O1	1b	(1/2,1/2,z)	(1/2,1/2,0.89730)
O2	2c	(1/2,0,z)	(1/2,0,0.37850) ; (0,1/2,0.37850)
Pb1	1a	(0,0,z)	(0,0,0)
Ti1	1b	(1/2,1/2,z)	(1/2,1/2,0.45170)

Structure 2

Space Group	*R3m* (160) with Z=3 (formula units per conventional unit cell)					
Cell parameters	**a**	5.7549	**b**	5.7549	**c**	7.1083
	α	90	**β**	90	**γ**	120

Atoms

ATOM	WP	Rep.	Orbit
O1	9b	(x,-x,z)	(0.82880,0.17120,0.60450) ; (0.82880,0.65760,0.60450) ; (0.34240,0.17120,0.60450) ; (0.49547,0.50453,0.93783) ; (0.49547,0.99093,0.93783) ; (0.00907,0.50453,0.93783) ; (0.16213,0.83787,0.27117) ; (0.16213,0.32427,0.27117) ; (0.67573,0.83787,0.27117)
Pb1	3a	(0,0,z)	(0,0,0) ; (2/3,1/3,1/3) ; (1/3,2/3,2/3)
Ti1	3a	(0,0,z)	(0,0,0.45950) ; (2/3,1/3,0.79283) ; (1/3,2/3,0.12617)

Attached copies: International Tables, Vol. A, with the Wyckoff positions of the space groups $P4mm$, $R3m$ and Cm;

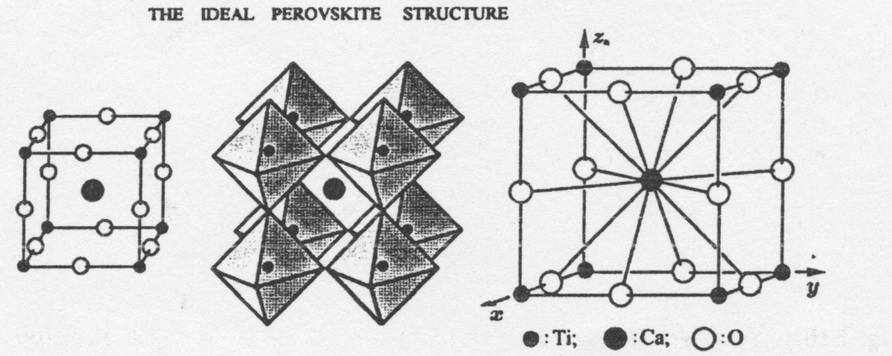
International Tables, Vol. A1, maximal-subgroup data and Wyckoff-positions splittings for the maximal subgroups of $R3m$.

1 EXERCISE: Phase Transitions of $BaTiO_3$

(T. Hahn, H. Wondratschek. *Symmetry in Crystals*. Sofia: Heron Press, 1994)

1.1 Problem

The crystal structure of $BaTiO_3$ is of perovskite type. Above 120C $BaTiO_3$ has the ideal paraelectric cubic structure (space group $P4/m\bar{3}2/m$) shown below. Below 120C $BaTiO_3$ assumes three structures with slightly deformed unit cells, all three being ferroelectric with different directions of the axis of spontaneous polarisation (polasr axis). The three ferroelectric polymorphs differ in the direction of displacement of the Ti-atoms from the centres of the octahedra:



Clinographic projection of the unit cell of the (idealized) cubic strucrure of perovskite, $CaTiO_3$

(a) No displacement: cubic structure

(b) Displacement parallel to a cube edge: <100>

(c) Displacement parallel to face diagonal of the cube: <110>

(d) Displacement parallel to a body diagonal of the cube: <111>.

1.2 Questions

(i) Which crystal systems and cell shapes result from the displacements (b) to (d)? Sketch outlines of the deformed unit cells with respect to the cubic cell.

(ii) Ferroelectricity requires a polar space group. Which space groups may the three polymorphs (b) to (d) have?

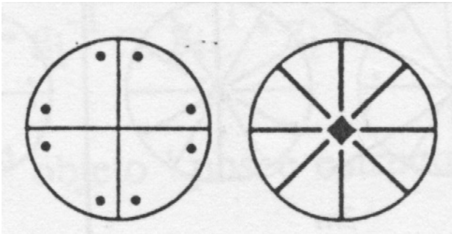
(iii) Which subgroup indices do these three space groups display with respect to the cubic group $Pm\bar{3}m$?

(iv) How many orientation states of the twin domains occur for each polymorph?
Which mutual orientation do the domains exhibit for case (b)?

2 EXERCISE: Subgroups of Point Group $4mm$; *Translationengleiche* Subgroups of Space Groups $P4mm$

2.1 Problem

(i) Derive from the stereographic projection of point $4mm$ all subgroups of indices [2] and [4].



(ii) Construct the complete subgroup diagram of point group $4mm$, see *Remark*.

(iii) Which of these subgroups are conjugate (symmetrically equivalent) in $4mm$ and which are normal subgroups?

(iv) Transfer the results from point group $4mm$ to space group $P4mm$ and its *translationengleiche* subgroups.

(v) Give the standard Hermann-Mauguin symbols of these subgroups.

Remark In a subgroup diagram each subgroup is located at a level which is determined y its index (the original group with index [1] on top, subgroups of index [2] nex lower level, *etc.*). Each of these groups is connected with its maximal subgroups by straight lines.

3 EXERCISE: Splitting of Wyckoff positions

3.1 Problem

Consider the group-subgroup pair $P4mm > Cm$, index 4. The relations between the conventional basis (**a**,**b**,**c**) of $P4mm$ and that of Cm (**a'**,**b'**,**c'**) (unique axis **b**, cell choice 1) are as follows: **a'**= -**a**-**b**, **b'**= **a**-**b**, **c'**= **c**.

For the $P4mm > Cm$, determine the splitting schemes of the Wyckoff positions $1a$, $1b$, $2c$ and $2d$ of $P4mm$.

Hint Transform the coordinates of the Wyckoff positions representatives of $P4mm$ to the subgroup basis, and then determine the splitting schemes by direct inspection.

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4	*b*	1	(1) x,y,z	(2) $x,\bar{y},z$	hkl : $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	*a*	*m*	$x,0,z$		

Symmetry of special projections

Along [001] $c\,1\,1\,m$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $C\,1$ ($P\,1$, 1) 1+

IIa [2] $P\,1\,a\,1$ ($P\,c$, 7) 1; $2+(\frac{1}{2},\frac{1}{2},0)$
[2] $P\,1\,m\,1$ ($P\,m$, 6) 1; 2

IIb [2] $C\,1\,c\,1$ ($\mathbf{c}'=2\mathbf{c}$) ($C\,c$, 9); [2] $I\,1\,c\,1$ ($\mathbf{c}'=2\mathbf{c}$) ($C\,c$, 9)

Maximal isomorphic subgroups of lowest index

IIc [2] $C\,1\,m\,1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{c},\mathbf{c}'=2\mathbf{c}$) ($C\,m$, 8); [3] $C\,1\,m\,1$ ($\mathbf{b}'=3\mathbf{b}$) ($C\,m$, 8)

Minimal non-isomorphic supergroups

I [2] $C\,2/m$ (12); [2] $C\,m\,m\,2$ (35); [2] $C\,m\,c\,2_1$ (36); [2] $A\,m\,m\,2$ (38); [2] $A\,e\,m\,2$ (39); [2] $F\,m\,m\,2$ (42); [2] $I\,m\,m\,2$ (44); [2] $I\,m\,a\,2$ (46); [3] $P\,3\,m\,1$ (156); [3] $P\,3\,1\,m$ (157); [3] $R\,3\,m$ (160)

II [2] $P\,1\,m\,1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P\,m$, 6)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			$hkl: h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2] $P4_2mc$ ($\mathbf{c}'=2\mathbf{c}$) (105); [2] $P4cc$ ($\mathbf{c}'=2\mathbf{c}$) (103); [2] $P4_2cm$ ($\mathbf{c}'=2\mathbf{c}$) (101); [2] $C4md$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4bm$, 100); [2] $F4mc$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4cm$, 108); [2] $F4mm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$) ($I4mm$, 107)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4mm$ ($\mathbf{c}'=2\mathbf{c}$) (99); [2] $C4mm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4mm$, 99)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

II [2] $I4mm$ (107)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	General:
18	c	1	(1) x,y,z (4) $\bar{y},\bar{x},z$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,z$	$hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$ Special: no extra conditions
9	b	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
3	a	$3m$	$0,0,z$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $R31$ ($R3$, 146) (1; 2; 3)+
{ [3] $R1m$ (Cm, 8) (1; 4)+
{ [3] $R1m$ (Cm, 8) (1; 5)+
{ [3] $R1m$ (Cm, 8) (1; 6)+

IIa [3] $P3m1$ (156) 1; 2; 3; 4; 5; 6

IIb [2] $R3c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (161)

Maximal isomorphic subgroups of lowest index

IIc [2] $R3m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=2\mathbf{c}$) (160); [4] $R3m$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (160)

Minimal non-isomorphic supergroups

I [2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

II [3] $P31m$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{3}\mathbf{c}$) (157)

$R3m$ No. 160 $R3m$ C_{3v}^5

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18 c 1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$
	(4) $\bar{y},\bar{x},z$ (5) $\bar{x}+y,y,z$ (6) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	(1; 2; 3)+		
{ [3] $R1m$ (8, $C1m1$)	(1; 4)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $R1m$ (8, $C1m1$)	(1; 5)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
{ [3] $R1m$ (8, $C1m1$)	(1; 6)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3m1$ (156)	1; 2; 3; 4; 5; 6		

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}'=\mathbf{a}+\mathbf{b}$, $\mathbf{b}'=-\mathbf{a}$, $\mathbf{c}'=2\mathbf{c}$			
$R3c$ (161)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a}+\mathbf{b},-\mathbf{a},2\mathbf{c}$	
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
{ $R3m$ (160)	$\langle 2;\ 4\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $R3m$ (160)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,0
{ $R3m$ (160)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	0,1,0
{ $R3m$ (160)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$ $p>1$; $p\equiv 2$ (mod 3) no conjugate subgroups	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	
$R3m$ (160)	$\langle 2;\ 4\rangle$ $p>6$; $p\equiv 1$ (mod 3) no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$			
$R3m$ (160)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$R3m$ (160)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>6$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1$ (mod 3)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P31m$ (157)

$R3m$ No. 160 C_{3v}^5

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions 3*a*	9*b*	18*c*
I Maximal *translationengleiche* subgroups					
[2] $R3$ (146)			$3a$	$9b$	$2\times 9b$
[3] $C1m1$ (8)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, -\frac{1}{2}x+y, x+z$	$2a$	$2a$; $4b$	$3\times 4b$
conjugate:	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}x+\frac{1}{2}y-z, -\frac{1}{2}x-\frac{1}{2}y, -x+y+z$			
conjugate:	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}y-z, x-\frac{1}{2}y, -y+z$			
alternative:	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \mathbf{c}$	$\frac{3}{2}x, -\frac{1}{2}x+y, x+z$			
or	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{3}{2}(-x+y), -\frac{1}{2}(x+y), -x+y+z$			
or	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \mathbf{c}$	$-\frac{3}{2}y, x-\frac{1}{2}y, -y+z$			
alternative:	$2\mathbf{a}+\mathbf{b}, -\mathbf{b}, -\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, \frac{1}{2}x-y, -3z$			
or	$-\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{b}, \frac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\frac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$\frac{1}{2}(-x+y)-z, \frac{1}{2}(x+y), -3z$			
or	$-\mathbf{a}-2\mathbf{b}, -\mathbf{a}, \frac{1}{3}(\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$-\frac{1}{2}y-z, -x+\frac{1}{2}y, -3z$			
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[3] $P3m1$ (156)			$1a$; $1b$; $1c$	$3\times 3d$	$3\times 6e$
Enlarged unit cell, non-isomorphic					
[2] $R3c$ (161)	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$6a$	$18b$	$2\times 18b$
Enlarged unit cell, isomorphic					
[2] $R3m$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times 3a$	$2\times 9b$	$2\times 18c$
[p] $R3m$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$	$-x, -y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times 3a$	$p\times 9b$	$p\times 18c$
	p = prime $= 3n-1$; $u = 1,\ldots,p-1$				
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$			
	p = prime $= 6n+1$; $u = 1,\ldots,p-1$				
[4] $R3m$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$3a$; $9b$	$2\times 9b$; $18c$	$4\times 18c$
[p^2] $R3m$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$	$-\frac{1}{p}x, -\frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$3a$; $(p-1)\times 9b$; $\frac{(p-1)(p-2)}{6}\times 18c$	$p\times 9b$; $\frac{p(p-1)}{2}\times 18c$	$p^2\times 18c$
	p = prime $= 3n-1$; $u, v = 1,\ldots,p-1$				
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$			
	p = prime $= 6n+1$; $u, v = 1,\ldots,p-1$				