SYMMETRY-MODE ANALYSIS
EXERCISES

Exercise 1. Identity symmetry modes

Determine the identity symmetry modes for an orbit of atoms belonging to the Wyckoff position 6*h* of $P6_3/mmc$;
How many independent displacive modes exist for the Wyckoff position 2*l*?
And for the Wyckoff position 2*a* ?

Necessary material: Table of the Wyckoff positions of $P6_3/mmc$ (p.601 of *IT*A)

Exercise 2. Chain-adapted modes for a group-subgroup chain with a maximal subgroup

(i)Consider the chain $P6_3/mmc > P\bar{3}m1$ of index 2. Determine the chain-adapted symmetry modes for an orbit of atoms belonging to the Wyckoff position 6*h* of $P6_3/mmc$;

Necessary material:
Wyckoff positions of $P\bar{3}m1$ (p.541 of *IT*A);
Maximal subgroups of $P6_3/mmc$ (p. 345 of *IT*A1);
Wyckoff-position splittings of $P6_3/mmc$ (p. 677 of *IT*A1).

(ii)Consider the chain $P\bar{3}m1$ > C2/m of index 3. Determine the chain-adapted symmetry modes for an orbit of atoms belonging to the Wyckoff position 6*i* of $P\bar{3}m1$.

Necessary material:
Wyckoff positions of *C*2/*m* (p.169 of *IT*A);
Maximal subgroups of $P\bar{3}m1$ (p. 309 of *IT*A1);
Wyckoff-position splittings of $P\bar{3}m1$ (p. 648 of *IT*A1).

Exercise 3. Chain-adapted modes for the symmetry break $P6_3/mmc$ > $C2/m$ (optional)

(i)Determine the graph of maximal subgroups for the symmetry break $P6_3/mmc > C2/m$ of index 6.

Necessary material:
Wyckoff positions of *Cmcm* (p.301 of *IT*A);
Maximal subgroups of *Cmcm* (p. 177 of *IT*A1);
Wyckoff-position splittings of *Cmcm* (p. 531 of *IT*A1).

(ii)Determine the Wyckoff position splitting diagrams for $P6_3/mmc > C2/m$ for atoms occupying 2*a*, 2*d* and 6*h*-orbits of $P6_3/mmc$. Determine the number and the symmetry of the corresponding primary and secondary modes.
(iii)Determine the chain-adapted modes for the atoms occupying 2*d* orbit of $P6_3/mmc$.

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	$hkl: h+k=2n$ $h0l: h=2n$ $0kl: k=2n$ $hk0: h+k=2n$ $0k0: k=2n$ $h00: h=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			$hkl: h=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			$hkl: h=2n$
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
- [2] $C1m1$ (Cm, 8) — (1; 4)+
- [2] $C121$ ($C2$, 5) — (1; 2)+
- [2] $C\bar{1}$ ($P\bar{1}$, 2) — (1; 3)+

IIa
- [2] $P12_1/a1$ ($P2_1/c$, 14) — 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
- [2] $P12/a1$ ($P2/c$, 13) — 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
- [2] $P12_1/m1$ ($P2_1/m$, 11) — 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
- [2] $P12/m1$ ($P2/m$, 10) — 1; 2; 3; 4

IIb [2] $C12/c1$ ($\mathbf{c}'=2\mathbf{c}$) ($C2/c$, 15); [2] $I12/c1$ ($\mathbf{c}'=2\mathbf{c}$) ($C2/c$, 15)

Maximal isomorphic subgroups of lowest index

IIc [2] $C12/m1$ ($\mathbf{c}'=2\mathbf{c}$ or $\mathbf{a}'=\mathbf{a}+2\mathbf{c},\mathbf{c}'=2\mathbf{c}$) ($C2/m$, 12); [3] $C12/m1$ ($\mathbf{b}'=3\mathbf{b}$) ($C2/m$, 12)

Minimal non-isomorphic supergroups

I [2] $Cmcm$ (63); [2] $\underline{C}mce$ (64); [2] $C\underline{m}mm$ (65); [2] $C\underline{m}me$ (67); [2] $Fmmm$ (69); [2] $Immm$ (71); [2] $Ibam$ (72); [2] $Imma$ (74); [2] $I4/m$ (87); [3] $P\bar{3}1m$ (162); [3] $P\bar{3}m1$ (164); [3] $R\bar{3}m$ (166)

II [2] $P12/m1$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/m$, 10)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
16	h	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	g	$..m$	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$	no extra conditions
8	f	$m..$	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$	$0,y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	e	$2..$	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$\bar{x},0,0$	$x,0,\frac{1}{2}$	hkl : $l=2n$
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl : $k,l=2n$
4	c	$m2m$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	b	$2/m..$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $l=2n$
4	a	$2/m..$	$0,0,0$	$0,0,\frac{1}{2}$			hkl : $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $C2cm$ ($Ama2$, 40)	(1; 4; 6; 7)+
	[2] $Cm2m$ ($Amm2$, 38)	(1; 3; 6; 8)+
	[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+
	[2] $C222_1$ (20)	(1; 2; 3; 4)+
	[2] $C12/c1$ ($C2/c$, 15)	(1; 3; 5; 7)+
	[2] $C2/m11$ ($C2/m$, 12)	(1; 4; 5; 8)+
	[2] $C112_1/m$ ($P2_1/m$, 11)	(1; 2; 5; 6)+
IIa	[2] $Pbnm$ ($Pnma$, 62)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcn$ ($Pnma$, 62)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcn$ (60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnm$ ($Pmmn$, 59)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmnn$ ($Pnnm$, 58)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbcm$ (57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pbnn$ ($Pnna$, 52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$
	[2] $Pmcm$ ($Pmma$, 51)	1; 2; 3; 4; 5; 6; 7; 8
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Cmcm$ ($\mathbf{a}'=3\mathbf{a}$) (63); [3] $Cmcm$ ($\mathbf{b}'=3\mathbf{b}$) (63); [3] $Cmcm$ ($\mathbf{c}'=3\mathbf{c}$) (63)

Minimal non-isomorphic supergroups

I [3] $P6_3/mcm$ (193); [3] $P6_3/mmc$ (194)

II [2] $Fmmm$ (69); [2] $Pmcm$ ($\mathbf{a}'=\frac{1}{2}\mathbf{a},\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($Pmma$, 51); [2] $Cmmm$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (65)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	j	1	(1) x,y,z (4) $y,x,\bar{z}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $\bar{y},\bar{x},z$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{x}+y,y,z$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$ (9) $x-y,x,\bar{z}$ (12) $x,x-y,z$				no conditions
									Special: no extra conditions
6	i	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$	
6	h	$.2.$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	g	$.2.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
3	f	$.2/m.$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	e	$.2/m.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	d	$3m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$					
2	c	$3m.$	$0,0,z$	$0,0,\bar{z}$					
1	b	$\bar{3}m.$	$0,0,\frac{1}{2}$						
1	a	$\bar{3}m.$	$0,0,0$						

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

Maximal non-isomorphic subgroups

I [2] $P3m1$ (156) 1; 2; 3; 10; 11; 12
[2] $P321$ (150) 1; 2; 3; 4; 5; 6
[2] $P\bar{3}11$ ($P\bar{3}$, 147) 1; 2; 3; 7; 8; 9
{ [3] $P12/m1$ ($C2/m$, 12) 1; 4; 7; 10
{ [3] $P12/m1$ ($C2/m$, 12) 1; 5; 7; 11
{ [3] $P12/m1$ ($C2/m$, 12) 1; 6; 7; 12

IIa none

IIb [2] $P\bar{3}c1$ ($\mathbf{c}'=2\mathbf{c}$) (165); [3] $H\bar{3}m1$ ($\mathbf{a}'=3\mathbf{a},\mathbf{b}'=3\mathbf{b}$) ($P\bar{3}1m$, 162)

Maximal isomorphic subgroups of lowest index

IIc [2] $P\bar{3}m1$ ($\mathbf{c}'=2\mathbf{c}$) (164); [4] $P\bar{3}m1$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) (164)

Minimal non-isomorphic supergroups

I [2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II [3] $H\bar{3}m1$ ($P\bar{3}1m$, 162); [3] $R\bar{3}m$ (obverse) (166); [3] $R\bar{3}m$ (reverse) (166)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$				
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$				
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$				
			(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
12	k	$.\,m\,.$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z+\frac{1}{2}$			no extra conditions
			$2x,x,z+\frac{1}{2}$	$\bar{x},x,z+\frac{1}{2}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$			
			$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$x,2x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$			
12	j	$m\,.\,.$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
			$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	$\bar{y},\bar{x},\frac{1}{4}$	$\bar{x}+y,y,\frac{1}{4}$	$x,x-y,\frac{1}{4}$	
12	i	$.\,2\,.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$hkil$: $l=2n$
			$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
6	h	$m\,m\,2$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
6	g	$.\,2/m\,.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3\,m\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3\,m\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					
2	b	$\bar{6}\,m\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	$\bar{3}\,m\,.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

(*Continued on preceding page*)

D_{2h}^{17} $C2/m2/c2_1/m$ No. 63 $Cmcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $C2cm$ (40, $Ama2$)	$\langle 1;\ 4;\ 6;\ 7\rangle+$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Cm2m$ (38, $Amm2$)	$\langle 1;\ 3;\ 6;\ 8\rangle+$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $Cmc2_1$ (36)	$\langle 1;\ 2;\ 7;\ 8\rangle+$		
[2] $C222_1$ (20)	$\langle 1;\ 2;\ 3;\ 4\rangle+$		
[2] $C12/c1$ (15)	$\langle 1;\ 3;\ 5;\ 7\rangle+$		
[2] $C2/m11$ (12, $C12/m1$)	$\langle 1;\ 4;\ 5;\ 8\rangle+$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112_1/m$ (11, $P112_1/m$)	$\langle 1;\ 2;\ 5;\ 6\rangle+$	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbnm$ (62, $Pnma$)	$1;\ 2;\ 5;\ 6;\ (3;\ 4;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pmcn$ (62, $Pnma$)	$1;\ 2;\ 7;\ 8;\ (3;\ 4;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $Pbcn$ (60)	$1;\ 3;\ 5;\ 7;\ (2;\ 4;\ 6;\ 8)+(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pmnm$ (59, $Pmmn$)	$1;\ 3;\ 6;\ 8;\ (2;\ 4;\ 5;\ 7)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $Pmnn$ (58, $Pnnm$)	$1;\ 4;\ 5;\ 8;\ (2;\ 3;\ 6;\ 7)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pbcm$ (57)	$1;\ 4;\ 6;\ 7;\ (2;\ 3;\ 5;\ 8)+(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$
[2] $Pbnn$ (52, $Pnna$)	$1;\ 2;\ 3;\ 4;\ (5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,0$
[2] $Pmcm$ (51, $Pmma$)	$1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8$	$\mathbf{c},\mathbf{a},\mathbf{b}$	

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Cmcm$ (63)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Cmcm$ (63)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cmcm$ (63)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Cmcm$ (63)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Cmcm$ (63)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Cmcm$ (63)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

D_{3d}^3 $\quad P\bar{3}2/m1$ $\quad$ No. 164 $\quad P\bar{3}m1$

Generators selected $(1);\ t(1,0,0);\ t(0,1,0);\ t(0,0,1);\ (2);\ (4);\ (7)$

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	j	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $P3m1$ (156)	1; 2; 3; 10; 11; 12	
[2] $P321$ (150)	1; 2; 3; 4; 5; 6	
[2] $P\bar{3}11$ (147, $P\bar{3}$)	1; 2; 3; 7; 8; 9	
{ [3] $P12/m1$ (12, $C12/m1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $P12/m1$ (12, $C12/m1$)	1; 5; 7; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$
{ [3] $P12/m1$ (12, $C12/m1$)	1; 6; 7; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{3}c1$ (165)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}c1$ (165)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{3}m1$ (164)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{3}m1$ (164)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{3}m1$ (164)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{3}m1$ (164)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{3}m1$ (162, $P\bar{3}1m$); [3] $R_{\mathrm{obv}}\bar{3}m$ (166, $R\bar{3}m$); [3] $R_{\mathrm{rev}}\bar{3}m$ (166, $R\bar{3}m$)

- **Decreased unit cell** $\quad$ none

D_{6h}^4 $\quad P6_3/m2/m2/c \quad$ No. 194 $\quad P6_3/mmc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates					
24 l 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
	(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$
	(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
	(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$	(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}2c$ (190)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24		
[2] $P\bar{6}m2$ (187)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21		$0,0,1/4$
[2] $P6_3mc$ (186)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24		
[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[2] $P6_3/m11$ (176, $P6_3/m$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18		
[2] $P\bar{3}m1$ (164)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21		
[2] $P\bar{3}1c$ (163)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24		
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 7; 10; 13; 16; 19; 22	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 8; 11; 13; 16; 20; 23	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 9; 12; 13; 16; 21; 24	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P6_3/mmc$ (194)	$\langle 2;\ 7;\ 13;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,1);\ (7;\ 13)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,1);\ (7;\ 13)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_3/mmc$ (194)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_3/mmc$ (194)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_3/mmc$ (194)	$\langle 2+(1,2,0);\ (4;\ 13)+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_3/mmc$ (194)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2});\ (7;\ 13)+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3/mmc$ (194)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 13)+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H6_3/mmc$ (193, $P6_3/mcm$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6/mmm$ (191)

	Axes	Coordinates	$4a$	$4b$	$4c$	$8d$	$8e$	$8f$	$8g$	$16h$
I Maximal *translationengleiche* subgroups										
[2] $C2cm$ (40) $\widehat{=}$ $Ama2$	$\mathbf{c}, \mathbf{b}, -\mathbf{a}$	$z,y,-x$	$4a$	$4a$	$4b$	$8c$	$2\times 4a$	$8c$	$2\times 4b$	$2\times 8c$
[2] $Cm2m$ (38) $\widehat{=}$ $Amm2$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$x,y,z+\frac{1}{4}$; $z+\frac{1}{4},x,y$	$4c$	$4c$	$2a$; $2b$	$8f$	$8f$	$2\times 4c$	$4d$; $4e$	$2\times 8f$
[2] $Cmc2_1$ (36)			$4a$	$4a$	$4a$	$8b$	$8b$	$2\times 4a$	$8b$	$2\times 8b$
[2] $C222_1$ (20)			$4a$	$4a$	$4b$	$8c$	$2\times 4a$	$8c$	$8c$	$2\times 8c$
[2] $C12/c1$ (15)			$4a$	$4b$	$4e$	$4c$; $4d$	$8f$	$8f$	$8f$	$2\times 8f$
[2] $C2/m11$ (12) $\widehat{=}$ $C12/m1$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y,-x,z$	$2a$; $2c$	$2b$; $2d$	$4i$	$4e$; $4f$	$4g$; $4h$	$2\times 4i$	$8j$	$2\times 8j$
[2] $P112_1/m$ (11)	$\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x+y,2y,z$	$2a$	$2c$	$2e$	$2b$; $2d$	$4f$	$4f$	$2\times 2e$	$2\times 4f$
	or: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$2x,x+y,z$	$2a$	$2b$	$2e$	$2c$; $2d$	$4f$	$4f$	$2\times 2e$	$2\times 4f$
	or: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y,x+y,z$	$2a$	$2d$	$2e$	$2b$; $2c$	$4f$	$4f$	$2\times 2e$	$2\times 4f$
II Maximal *klassengleiche* subgroups										
Loss of centering translations										
[2] $Pbnm$ (62) $\widehat{=}$ $Pnma$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y,z,x	$4a$	$4b$	$4c$	$8d$	$8d$	$8d$	$2\times 4c$	$2\times 8d$
[2] $Pmcn$ (62) $\widehat{=}$ $Pnma$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$x+\frac{1}{4},y+\frac{1}{4},z$; $z,x+\frac{1}{4},y+\frac{1}{4}$	$4c$	$4c$	$4c$	$4a$; $4b$	$8d$	$2\times 4c$	$8d$	$2\times 8d$
[2] $Pbcn$ (60)			$4a$	$4b$	$4c$	$8d$	$8d$	$8d$	$8d$	$2\times 8d$
[2] $Pmnm$ (59) $\widehat{=}$ $Pmmn$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	origin 1: $x,y+\frac{1}{4},z+\frac{1}{4}$; origin 2: $x-\frac{1}{4},y+\frac{1}{4},z$; $z+\frac{1}{4},x,y+\frac{1}{4}$ (origin 1); $z,x-\frac{1}{4},y+\frac{1}{4}$ (origin 2)	$4f$	$4f$	$2a$; $2b$	$4c$; $4d$	$8g$	$2\times 4f$	$2\times 4e$	$2\times 8g$
[2] $Pmnn$ (58) $\widehat{=}$ $Pnnm$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y,z,x	$2a$; $2c$	$2b$; $2d$	$4g$	$8h$	$4e$; $4f$	$2\times 4g$	$8h$	$2\times 8h$
[2] $Pbcm$ (57)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4c$	$4c$	$4d$	$4a$; $4b$	$2\times 4c$	$8e$	$2\times 4d$	$2\times 8e$
[2] $Pbnn$ (52) $\widehat{=}$ $Pnna$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$x+\frac{1}{4},y+\frac{1}{4},z$; $y+\frac{1}{4},z,x+\frac{1}{4}$	$4c$	$4c$	$4d$	$4a$; $4b$	$2\times 4c$	$8e$	$8e$	$2\times 8e$
[2] $Pmcm$ (51) $\widehat{=}$ $Pmma$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z,x,y	$2a$; $2d$	$2b$; $2c$	$2e$; $2f$	$8l$	$4g$; $4h$	$4i$; $4j$	$2\times 4k$	$2\times 8l$
Enlarged unit cell, isomorphic										
[3] $Cmcm$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$4a$; $8e$	$4b$; $8e$	$4c$; $8g$	$8d$; $16h$	$3\times 8e$	$8f$; $16h$	$3\times 8g$	$3\times 16h$
[p] $Cmcm$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$; p = prime > 2; $u = 1,\ldots,p-1$	$\frac{1}{3}x,y,z$; $+(\frac{u}{p},0,0)$	$4a$; $\frac{p-1}{2}\times 8e$	$4b$; $\frac{p-1}{2}\times 8e$	$4c$; $\frac{p-1}{2}\times 8g$	$8d$; $\frac{p-1}{2}\times 16h$	$p\times 8e$	$8f$; $\frac{p-1}{2}\times 16h$	$p\times 8g$	$p\times 16h$
[3] $Cmcm$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$4a$; $8f$	$4b$; $8f$	$3\times 4c$	$8d$; $16h$	$8e$; $16h$	$3\times 8f$	$3\times 8g$	$3\times 16h$
[p] $Cmcm$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$; p = prime > 2; $u = 1,\ldots,p-1$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$4a$; $\frac{p-1}{2}\times 8f$	$4b$; $\frac{p-1}{2}\times 8f$	$p\times 4c$	$8d$; $\frac{p-1}{2}\times 16h$	$8e$; $\frac{p-1}{2}\times 16h$	$p\times 8f$	$p\times 8g$	$p\times 16h$
[3] $Cmcm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a$; $8f$	$4b$; $8f$	$4c$; $8f$	$8d$; $16h$	$8e$; $16h$	$3\times 8f$	$8g$; $16h$	$3\times 16h$
[p] $Cmcm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; p = prime > 2; $u = 1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a$; $\frac{p-1}{2}\times 8f$	$4b$; $\frac{p-1}{2}\times 8f$	$4c$; $\frac{p-1}{2}\times 8f$	$8d$; $\frac{p-1}{2}\times 16h$	$8e$; $\frac{p-1}{2}\times 16h$	$p\times 8f$	$8g$; $\frac{p-1}{2}\times 16h$	$p\times 16h$

Continued on preceding page

$P\bar{3}m1$ No. 164 $P\bar{3}2/m1$ D_{3d}^{3}

	Axes	Coordinates	Wyckoff positions					
			$1a$	$1b$	$2c$ $6g$	$2d$ $6h$	$3e$ $6i$	$3f$ $12j$
I Maximal *translationengleiche* subgroups								
[2] $P3m1$ (156)			$1a$	$1a$	$2\times1a$ $6e$	$1b;1c$ $6e$	$3d$ $2\times3d$	$3d$ $2\times6e$
[2] $P321$ (150)			$1a$	$1b$	$2c$ $2\times3e$	$2d$ $2\times3f$	$3e$ $6g$	$3f$ $2\times6g$
[2] $P\bar{3}$ (147)			$1a$	$1b$	$2c$ $6g$	$2d$ $6g$	$3e$ $6g$	$3f$ $2\times6g$
[3] $C12/m1$ (12)	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a$	$2c$	$4i$ $4g; 8j$	$4i$ $4h; 8j$	$2b; 4e$ $4i; 8j$	$2d; 4f$ $3\times8j$
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$ $(\frac{1}{2},\frac{1}{2},0)$						
conjugate:	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z;$ $+(\frac{1}{2},\frac{1}{2},0)$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, nonisomorphic								
[2] $P\bar{3}c1$ (165)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$2b$	$2a$	$4c$ $12g$	$4d$ $2\times6f$	$6e$ $12g$	$6f$ $2\times12g$
[2] $P\bar{3}c1$ (165)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$ $2\times6f$	$4d$ $12g$	$6f$ $12g$	$6e$ $2\times12g$
[3] $P\bar{3}1m$ (162)	$2\mathbf{a}+\mathbf{b},$ $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y),$ $z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a; 2c$	$1b; 2d$	$2e; 4h$ $3\times6i$	$6k$ $3\times6j$	$3f; 6i$ $6k; 12l$	$3g; 6j$ $3\times12l$
Enlarged unit cell, isomorphic								
[2] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$1a; 1b$	$2c$	$2\times2c$ $6g; 6h$	$2\times2d$ $12j$	$3e; 3f$ $2\times6i$	$6i$ $2\times12j$
[2] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$2c$	$1a; 1b$	$2\times2c$ $12j$	$2\times2d$ $6g; 6h$	$6i$ $2\times6i$	$3e; 3f$ $2\times12j$
[3] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$1a; 2c$	$1b; 2c$	$3\times2c$ $6g; 12j$	$3\times2d$ $6h; 12j$	$3e; 6i$ $3\times6i$	$3f; 6i$ $3\times12j$
[p] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2;$ $u = 1, \dots, p-1$	$x, y, \frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$1a; \frac{p-1}{2}\times2c$	$1b; \frac{p-1}{2}\times2c$	$p\times2c$ $6g; \frac{p-1}{2}\times12j$	$p\times2d$ $6h; \frac{p-1}{2}\times12j$	$3e; \frac{p-1}{2}\times6i$ $p\times6i$	$3f; \frac{p-1}{2}\times6i$ $p\times12j$
[4] $P\bar{3}m1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3e$	$1b; 3f$	$2c; 6i$ $2\times6g; 12j$	$2d; 6i$ $2\times6h; 12j$	$6g; 6i$ $2\times6i; 12j$	$6h; 6i$ $4\times12j$
[p^2] $P\bar{3}m1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 4;$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ $u, v = 1, \dots, p-1$	$1a; \frac{p-1}{2}\times6g;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)(p-5)}{12}\times$ $12j$	$1b; \frac{p-1}{2}\times6h;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)(p-5)}{12}\times$ $12j$	$2c;$ $(p-1)\times6i;$ $\frac{(p-1)(p-2)}{6}\times$ $12j$ $p\times6g;$ $\frac{p(p-1)}{2}\times12j$	$2d;$ $(p-1)\times6i;$ $\frac{(p-1)(p-2)}{6}\times$ $12j$ $p\times6h;$ $\frac{p(p-1)}{2}\times12j$	$3e; \frac{p-1}{2}\times6g;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)^2}{4}\times12j$ $p\times6i;$ $\frac{p(p-1)}{2}\times12j$	$3f; \frac{p-1}{2}\times6h;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)^2}{4}\times12j$ $p^2\times12i$

D_{6h}^{4} $\quad P6_3/m2/m2/c$ $\quad$ No. 194 $\quad P6_3/mmc$

	Axes	Coordinates	Wyckoff positions					
			$2a$ $6g$	$2b$ $6h$	$2c$ $12i$	$2d$ $12j$	$4e$ $12k$	$4f$ $24l$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}2c$ (190)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{6}m2$ (187)		$x,y,z+\frac{1}{4}$	$2g$ $6n$	$1a$; $1b$ $3j$; $3k$	$1d$; $1e$ $12o$	$1c$; $1f$ $6l$; $6m$	$2\times2g$ $2\times6n$	$2h$; $2i$ $2\times12o$
[2] $P6_3mc$ (186)			$2a$ $6c$	$2a$ $6c$	$2b$ $12d$	$2b$ $12d$	$2\times2a$ $2\times6c$	$2\times2b$ $2\times12d$
[2] $P6_322$ (182)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P6_3/m$ (176)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{3}m1$ (164)			$1a$; $1b$ $3e$; $3f$	$2c$ $6i$	$2d$ $6g$; $6h$	$2d$ $12j$	$2\times2c$ $2\times6i$	$2\times2d$ $2\times12j$
[2] $P\bar{3}1c$ (163)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[3] $Cmcm$ (63)	$\mathbf{a}$, $\mathbf{a}+2\mathbf{b}$, $\mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$; $+(\frac{1}{2},\frac{1}{2},0)$	$4a$ $4b$; $8d$	$4c$ $4c$; $8g$	$4c$ $8e$; $16h$	$4c$ $3\times8g$	$8f$ $8f$; $16h$	$8f$ $3\times16h$
conjugate:	$\mathbf{b}$, $-2\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$; $+(\frac{1}{2},\frac{1}{2},0)$						
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$; $+(\frac{1}{2},\frac{1}{2},0)$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, nonisomorphic								
[3] $P6_3/mcm$ (193)	$\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y)$, z; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2b$; $4d$ $6f$; $12i$	$2a$; $4c$ $6g$; $12j$	$6g$ $3\times12i$	$6g$ $3\times12j$	$4e$; $8h$ $12k$; $24l$	$12k$ $3\times24l$
Enlarged unit cell, isomorphic								
[3] $P6_3/mmc$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$ $6g$; $12k$	$2b$; $4e$ $6h$; $12k$	$2d$; $4f$ $12i$; $24l$	$2c$; $4f$ $12j$; $24l$	$3\times4e$ $3\times12k$	$3\times4f$ $3\times24l$
[p] $P6_3/mmc$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$ $p=$ prime >2;	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u=1\ldots p-1$	$2a$; $\frac{p-1}{2}\times4e$ $6g$; $\frac{p-1}{2}\times12k$	$2b$; $\frac{p-1}{2}\times4e$ $6h$; $\frac{p-1}{2}\times12k$	$2c(d^*)$; $\frac{p-1}{2}\times4f$ $12i$; $\frac{p-1}{2}\times24l$	$2d(c^*)$; $\frac{p-1}{2}\times4f$ $12j$; $\frac{p-1}{2}\times24l$	$p\times4e$ $p\times12k$	$p\times4f$ $p\times24l$
[4] $P6_3/mmc$	$2\mathbf{a}$, $2\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6g$ $12i$; $12k$	$2b$; $6h$ $2\times6h$; $12j$	$2d$; $6h$ $2\times12i$; $24l$	$2c$; $6h$ $4\times12j$	$4e$; $12k$ $2\times12k$; $24l$	$4f$; $12k$ $4\times24l$
[p^2] $P6_3/mmc$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ $p=$ prime >4;	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)(p-5)}{12}\times24l$ $6g$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)^2}{4}\times24l$	$2b$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times6h$; $\frac{p(p-1)}{2}\times12j$	$2c(d^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times12i$; $\frac{p(p-1)}{2}\times24l$	$2d(c^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p^2\times12j$	$4e$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p\times12k$; $\frac{p(p-1)}{2}\times24l$	$4f$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p^2\times24l$

* $p=4n-1$ $\qquad$ † $p=6n-1$