

$\bar{6}3/mmc$

$6/mmm$

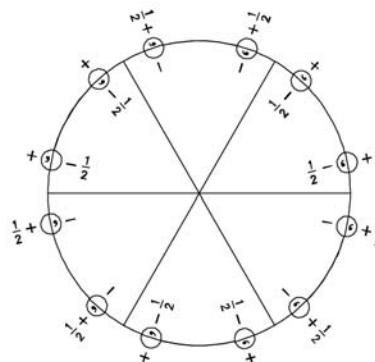
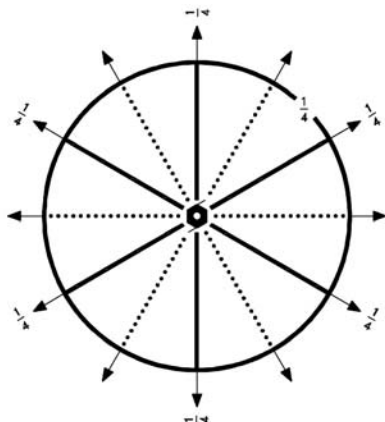
Hexagonal

No. 75

$\bar{6}3/m2/m2/c$

Patterson symmetry $\bar{6}3/mmm$

FIRST SETTING



Origin at centre ($\bar{3}m1$) at $\bar{3}2/mc$

Asymmetric unit $y \leq x/2; -x \leq y; 0 \leq z \leq \frac{1}{4}$

Symmetry operations

- | | | |
|--------------------------------|---|---|
| (1) 1 | (2) $3^+ 0,0,z$ | (3) $3^- 0,0,z$ |
| (4) $2(\frac{1}{2}) 0,0,z$ | (5) $6^-(\frac{1}{2}) 0,0,z$ | (6) $6^+(\frac{1}{2}) 0,0,z$ |
| (7) $2 x,x,0$ | (8) $2 x,0,0$ | (9) $2 0,y,0$ |
| (10) $2 x,\bar{x},\frac{1}{4}$ | (11) $2 x,2x,\frac{1}{4}$ | (12) $2 2x,x,\frac{1}{4}$ |
| (13) $\bar{1} 0,0,0$ | (14) $\bar{3}^+ 0,0,z; 0,0,0$ | (15) $\bar{3}^- 0,0,z; 0,0,0$ |
| (16) $m x,y,\frac{1}{4}$ | (17) $\bar{6}^- 0,0,z; 0,0,\frac{1}{4}$ | (18) $\bar{6}^+ 0,0,z; 0,0,\frac{1}{4}$ |
| (19) $m x,\bar{x},z$ | (20) $m x,2x,z$ | (21) $m 2x,x,z$ |
| (22) $c x,x,z$ | (23) $c x,0,z$ | (24) $c 0,y,z$ |

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

Positions

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

Special: no extra conditions

12 <i>g</i> . <i>m</i> .	$x, 2x, z$ $2x, x, \bar{z}$	$2\bar{x}, \bar{x}, z$ $\bar{x}, 2\bar{x}, \bar{z}$	x, \bar{x}, z \bar{x}, x, \bar{z}	$\bar{x}, 2\bar{x}, z + \frac{1}{2}$ $2\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$	$2x, x, z + \frac{1}{2}$ $x, 2x, \bar{z} + \frac{1}{2}$	$\bar{x}, x, z + \frac{1}{2}$ $x, \bar{x}, \bar{z} + \frac{1}{2}$
12 <i>f</i> <i>m</i> . .	$x, y, \frac{1}{4}$ $y, x, \frac{3}{4}$	$\bar{y}, x - y, \frac{1}{4}$ $x - y, \bar{y}, \frac{3}{4}$	$\bar{x} + y, \bar{x}, \frac{1}{4}$ $\bar{x}, \bar{x} + y, \frac{3}{4}$	$\bar{x}, \bar{y}, \frac{3}{4}$ $\bar{y}, \bar{x}, \frac{1}{4}$	$y, \bar{x} + y, \frac{3}{4}$ $\bar{x} + y, y, \frac{1}{4}$	$x - y, x, \frac{3}{4}$ $x, x - y, \frac{1}{4}$
12 <i>e</i> . 2 .	$x, 0, 0$ $\bar{x}, 0, 0$	$0, x, 0$ $0, \bar{x}, 0$	$\bar{x}, \bar{x}, 0$ $x, x, 0$	$\bar{x}, 0, \frac{1}{2}$ $x, 0, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$ $0, x, \frac{1}{2}$	$x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$
6 <i>d</i> <i>m m</i> 2	$x, 2x, \frac{1}{4}$	$2\bar{x}, \bar{x}, \frac{1}{4}$	$x, \bar{x}, \frac{1}{4}$	$\bar{x}, 2\bar{x}, \frac{3}{4}$	$2x, x, \frac{3}{4}$	$\bar{x}, x, \frac{3}{4}$
4 <i>c</i> 3 <i>m</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$	$0, 0, \bar{z}$	$0, 0, \bar{z} + \frac{1}{2}$		
2 <i>b</i> $\bar{6} m 2$	$0, 0, \frac{1}{4}$	$0, 0, \frac{3}{4}$				
2 <i>a</i> $\bar{3} m .$	$0, 0, 0$	$0, 0, \frac{1}{2}$				

Symmetry of special projections

Along [001] $6mm$

Along [100] $\bar{6}2mg$

Along [210] $\bar{6}2mm$

Origin at $0, 0, z$

$\mathbf{a}' = \mathbf{c}$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I [2] $\bar{6}2c$ ($\bar{6}c2, 72$)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
[2] $\bar{6}m2$ (71)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
[2] $\bar{6}_3mc$ (70)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
[2] $\bar{6}_322$ (65)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[2] $\bar{6}_3/m11$ ($\bar{6}_3/m, 61$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
[2] $\bar{3}1c$ (52)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
[2] $\bar{3}m1$ ($\bar{3}1m, 51$)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
[3] $\bar{6}mmc$ ($\bar{6}mcm, 22$)	1; 4; 7; 10; 13; 16; 19; 22
[3] $\bar{6}mmc$ ($\bar{6}mcm, 22$)	1; 4; 8; 11; 13; 16; 20; 23
[3] $\bar{6}mmc$ ($\bar{6}mcm, 22$)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc [3] $\bar{6}_3/mmc$ ($\mathbf{c}' = 3\mathbf{c}$) (75)

Minimal non-isotypic non-enantiomorphic supergroups

I none

II [2] $\bar{6}/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (73)

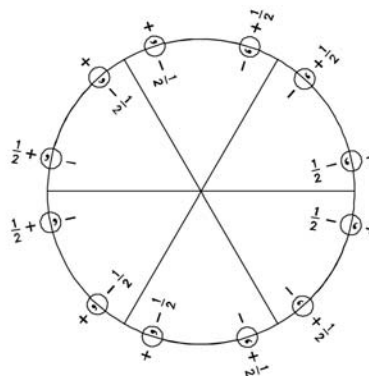
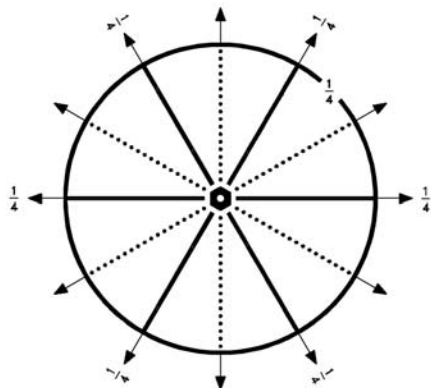
$\mu 6_3/mcm$ $6/mmm$

Hexagonal

No. 75

 $\mu 6_3/m2/c2/m$ Patterson symmetry $\mu 6/mmm$

SECOND SETTING

**Origin** at centre ($\bar{3}1m$) at $\bar{3}c2/m$ **Asymmetric unit** $0 \leq x$; $0 \leq y$; $0 \leq z \leq \frac{1}{4}$; $y \leq x$ **Symmetry operations**

- | | | |
|------------------------------|--|--|
| (1) 1 | (2) 3^+ $0,0,z$ | (3) 3^- $0,0,z$ |
| (4) $2(\frac{1}{2})$ $0,0,z$ | (5) $6^-(\frac{1}{2})$ $0,0,z$ | (6) $6^+(\frac{1}{2})$ $0,0,z$ |
| (7) 2 $x,x,\frac{1}{4}$ | (8) 2 $x,0,\frac{1}{4}$ | (9) 2 $0,y,\frac{1}{4}$ |
| (10) 2 $x,\bar{x},0$ | (11) 2 $x,2x,0$ | (12) 2 $2x,x,0$ |
| (13) $\bar{1}$ $0,0,0$ | (14) $\bar{3}^+$ $0,0,z$; $0,0,0$ | (15) $\bar{3}^-$ $0,0,z$; $0,0,0$ |
| (16) m $x,y,\frac{1}{4}$ | (17) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$ | (18) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$ |
| (19) c x,\bar{x},z | (20) c $x,2x,z$ | (21) c $2x,x,z$ |
| (22) m x,x,z | (23) m $x,0,z$ | (24) m $0,y,z$ |

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

Positions

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

Symmetry of special projections

Along [001] $6mm$

Along [100] $\mu 2mm$

Along [210] $\mu 2mg$

Origin at $0, 0, z$

$\mathbf{a}' = \frac{1}{2}\mathbf{c}$

Origin at $x, 0, 0$

$\mathbf{a}' = \mathbf{c}$

Origin at $x, \frac{1}{2}x, 0$

Maximal non-isotypic non-enantiomorphic subgroups

I	$[2]\mu\bar{6}c2$ (72)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21
	$[2]\mu\bar{6}2m$ ($\mu\bar{6}m2$, 71)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24
	$[2]\mu\bar{6}_3cm$ ($\mu\bar{6}_3mc$, 70)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24
	$[2]\mu\bar{6}_322$ (65)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	$[2]\mu\bar{6}_3/m11$ ($\mu\bar{6}_3/m$, 61)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18
	$[2]\mu\bar{3}c1$ ($\mu\bar{3}1c$, 52)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21
	$[2]\mu\bar{3}1m$ (51)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 7; 10; 13; 16; 19; 22
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 8; 11; 13; 16; 20; 23
	$[3]\mu mcm$ (μmcm , 22)	1; 4; 9; 12; 13; 16; 21; 24

IIa none

IIb none

Maximal isotypic subgroups and enantiomorphic subgroups of lowest index

IIc $[3]\mu\bar{6}_3/mcm$ ($\mathbf{c}' = 3\mathbf{c}$) ($\mu\bar{6}_3/mmc$, 75)

Minimal non-isotypic non-enantiomorphic supergroups

I none

II $[2]\mu\bar{6}/mmm$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (73)