

A brief conducted tour of some entries in International Tables for Crystallography, Volume A

$P 2_1 2_1 2_1$

D_2^4

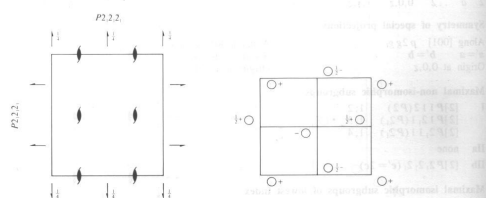
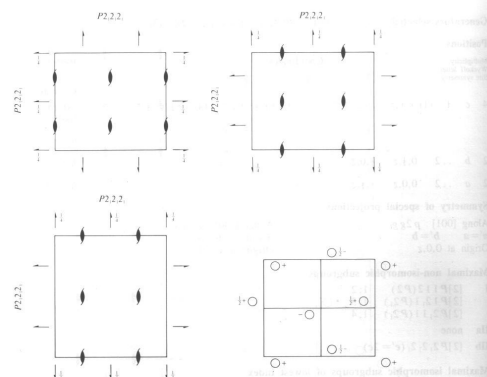
2 2 2

Orthorhombic

No. 19

$P 2_1 2_1 2_1$

Patterson symmetry $P m m m$



Origin at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,0,1) \perp 0,z$ (3) $2(0,1,0) \parallel 0,y,1$ (4) $2(1,0,0) \parallel x,1,0$

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

4 $a = 1$ (1) x,y,z (2) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$ (3) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$

Symmetry of special projections

Along $[001]$ $p 2gg$

$a' = a$ $b' = b$

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

Along $[100]$ $p 2gg$

$a' = b$ $b' = c$

Origin at $x,1,0$

Along $[010]$ $p 2gg$

$a' = c$ $b' = a$

Origin at $0,y,1$

Maximal non-isomorphic subgroups

I $[2]P 112, (P 2_1)$ 1; 2

$[2]P 12, 1(P 2_1)$ 1; 3

$[2]P 2, 11(P 2_1)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]P 2, 2, 2; (a' = 3a \text{ or } b' = 3b \text{ or } c' = 3c)$

Minimal non-isomorphic supergroups

I $[2]P bca; [2]P nm a; [2]P 4, 2, 2; [2]P 4, 2, 2; [3]P 2, 3$

II $[2]A 2, 2, 2(C 222); [2]B 2, 2, 2(C 222); [2]C 222; [2]I 2, 2, 2; [2]P 2, 2, 2; (2a' = a)(P 2, 2, 2); [2]P 2, 2, 2; (2b' = b)(P 2, 2, 2); [2]P 2, 2, 2; (2c' = c)$

$P 2_1/c$

C_{2h}^5

$2/m$

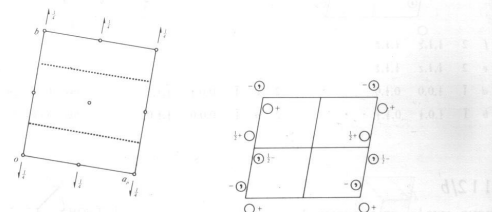
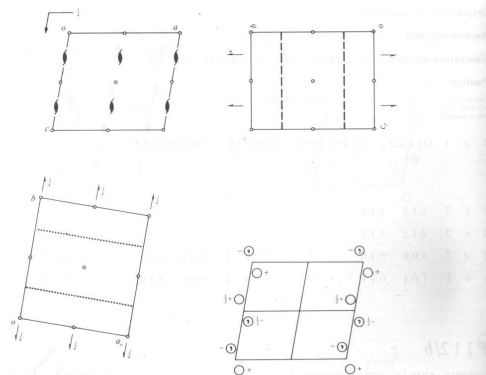
Monoclinic

No. 14

$P 12/c 1$

Patterson symmetry $P 12/m 1$

UNIQUE AXIS b , CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,1,0) \parallel 0,y,1$ (3) $\bar{1} \parallel 0,0,0$ (4) $c \parallel x,1,z$

CONTINUED	No. 14	$P2_1/c$
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)		
Positions	Coordinates	Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		
4 e 1 (1) x, y, z (2) $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$		General: $h0l: l=2n$ $0k0: k=2n$ $00l: l=2n$ Special: as above, plus $hkl: k+l=2n$ $hkl: k+l=2n$ $hkl: k+l=2n$ $hkl: k+l=2n$
Symmetry of special projections		
Along $[001]$ $p2gm$ $a'=a$ $b'=b$ Origin at $0,0,z$	Along $[100]$ $p2gg$ $a'=b$ $b'=c$ Origin at $x,0,0$	Along $[010]$ $p2$ $a'=c$ $b'=a$ Origin at $0,y,0$
Maximal non-isomorphic subgroups		
I $[2]P2_1, [1](P2_1)$ 1:2 $[2]P\bar{1}$ 1:3		

$R3c$	C_{3v}^6	$3m$	Trigonal
No. 161	$R3c$		Patterson symmetry $R\bar{3}m$
HEXAGONAL AXES			
Origin on $3c$			
Asymmetric unit $0 \leq x \leq \frac{1}{3}$; $0 \leq y \leq \frac{1}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$			
Vertices $0,0,0$ $\frac{1}{3},0,0$ $\frac{2}{3},0,0$ $0,\frac{1}{3},0$ $0,\frac{2}{3},0$ $0,0,\frac{1}{2}$			

Origin on $3c$		
Asymmetric unit $0 \leq x \leq \frac{1}{3}$; $0 \leq y \leq \frac{1}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq (1+y)/2$; $y \leq \min(1-x, (1+x)/2)$		
Vertices $0,0,0$ $\frac{1}{3},0,0$ $\frac{2}{3},0,0$ $0,\frac{1}{3},0$ $0,\frac{2}{3},0$ $0,0,\frac{1}{2}$		
Symmetry operations		
For $(0,0,0)+$ set		
(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) c x,x,z	(5) c $x,2x,z$	(6) c $2x,x,z$
For $(\frac{1}{3},\frac{1}{3},\frac{1}{2})+$ set		
(1) $t(\frac{1}{3},\frac{1}{3},\frac{1}{2})$	(2) $3^+(0,0,\frac{1}{2})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{2})$ $\frac{1}{3},\frac{1}{3},z$
(4) $g(\frac{1}{3},-\frac{1}{3},\frac{1}{2})$ $x+\frac{1}{3},\bar{x},z$	(5) $g(\frac{1}{3},\frac{1}{3},\frac{1}{2})$ $x,2x-\frac{1}{3},z$	(6) $g(\frac{1}{3},\frac{1}{3},\frac{1}{2})$ $2x,x,z$
For $(\frac{1}{3},\frac{1}{3},\frac{1}{2})+$ set		
(1) $t(\frac{1}{3},\frac{1}{3},\frac{1}{2})$	(2) $3^+(0,0,\frac{1}{2})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{2})$ $\frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{3},\frac{1}{3},\frac{1}{2})$ $x+\frac{1}{3},\bar{x},z$	(5) $g(\frac{1}{3},\frac{1}{3},\frac{1}{2})$ $x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{3},\frac{1}{2})$ $2x-\frac{1}{3},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{3},\frac{1}{3},\frac{1}{2})$; (2); (4)		
Positions	Coordinates	Reflection conditions
Multiplicity, Wyckoff letter, Site symmetry		
18 b 1 (1) x, y, z (2) \bar{x}, \bar{y}, z (3) $x+y, \bar{x}, z$ (4) $\bar{x}, \bar{y}, z+\frac{1}{2}$ (5) $x+y, y, z+\frac{1}{2}$ (6) $x, x-y, z+\frac{1}{2}$		General: $hkl: -h+k+l=3n$ $hkl0: -h+k=3n$ $hh2h: l=3n$ $hh0l: h+l=3n, l=2n$ $000l: l=6n$ $h000: h=3n$ Special: as above, plus $hkl: l=2n$
Symmetry of special projections		
Along $[001]$ $p31m$ $a'=1(2a+b)$ $b'=1(-a+b)$ $c'=1(2a+4b+c)$ $b'=1(-a-2b+c)$ Origin at $0,0,z$	Along $[100]$ $p1$ $a'=1(2a+4b+c)$ $b'=1(-a-2b+c)$ Origin at $x,0,0$	Along $[210]$ $p1g1$ $a'=1b$ $b'=1c$ Origin at $x,\frac{1}{2},0$
Maximal non-isomorphic subgroups		
I $[2]R\bar{3}1(R3)$ (1; 2; 3)+ $[3]R1c(Cc)$ (1; 4)+ $[3]R1c(Cc)$ (1; 5)+ $[3]R1c(Cc)$ (1; 6)+		
IIa $[3]P3c1$ 1; 2; 3; 4; 5; 6		
IIb none		
Maximal isomorphic subgroups of lowest index		
IIc $[5]R3c(a'=-a, b'=-b, c'=5c)$; $[4]R3c(a'=-2a, b'=-2b)$		
Minimal non-isomorphic supergroups		
I $[2]R3c$; $[4]P\bar{4}3n$; $[4]F\bar{4}3c$; $[4]I\bar{4}3d$		

...and now for something
(completely??) different...

Interactive space groups!