

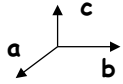
Reticolo cristallino

Il reticolo e' descritto da una base costituita da 3 vettori: $\vec{a}, \vec{b}, \vec{c}$

Ciascun punto reticolare \vec{Q} e' ottenibile dalla **combinazione lineare** dei vettori di base:

$$\vec{Q}_{uvw} = u\vec{a} + v\vec{b} + w\vec{c}$$

Se la cella elementare è **primitiva** (i.e. contiene un solo punto reticolare) u, v, w sono interi:



$$(u, v, w) \in \mathfrak{S}$$

Piani reticolari

Consideriamo un piano che intercetta i 3 assi cristallografici $\vec{a}, \vec{b}, \vec{c}$ nei punti: $(p, 0, 0), (0, q, 0), (0, 0, r)$

L'equazione del piano sarà (equazione di primo grado con 3 incognite $\Rightarrow \mathfrak{R}^2$ soluzioni \Rightarrow piano)

$$\frac{x}{p} + \frac{y}{q} + \frac{z}{r} = 1$$

Moltiplicando per $pqr=m \Rightarrow \quad qrx + pry + pqz = m \quad \Rightarrow \quad hx + ky + lz = m$

Variando m si ottiene una famiglia di **piani paralleli**

<http://escher.epfl.ch/eCrystallography/>

1

Coordinate di un punto nel piano $x_1, y_1, z_1 \rightarrow \frac{x_1}{p} + \frac{y_1}{q} + \frac{z_1}{r} = 1$

Coordinate di un vettore nel piano $x_1 - x_2, y_1 - y_2, z_1 - z_2$

$$\begin{cases} \frac{x_1}{p} + \frac{y_1}{q} + \frac{z_1}{r} = 1 \\ \frac{x_2}{p} + \frac{y_2}{q} + \frac{z_2}{r} = 1 \end{cases} \Rightarrow \frac{x_1 - x_2}{p} + \frac{y_1 - y_2}{q} + \frac{z_1 - z_2}{r} = 0$$

prodotto scalare

$$\frac{x_1 - x_2}{p} + \frac{y_1 - y_2}{q} + \frac{z_1 - y_2}{r} = \left(\frac{1}{p}, \frac{1}{q}, \frac{1}{r} \right) \cdot (x_1 - x_2, y_1 - y_2, z_1 - z_2) = 0$$

$\left(\frac{1}{p}, \frac{1}{q}, \frac{1}{r} \right) = (h, k, l)$ coordinate di un vettore perpendicolare al piano che interseca gli assi in p, q, r

2

$$hx + ky + lz = m$$

una terna di indici h, k, l definisce una famiglia di piani paralleli nel reticolo diretto e un punto nel **reticolo reciproco**: se si sceglie $m = 1$ allora il piano interseca gli assi reticolari nei punti

$$\left(\frac{1}{h}, \frac{1}{k}, \frac{1}{l}\right)$$

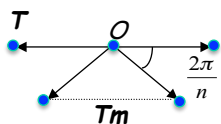
Gli indici h, k, l sono detti **indici di Miller**

simmetrie

Restrizioni alle **simmetrie possibili** dovute alla periodicit  del reticolo cristallino

rotazioni

Sia T un vettore di reticolo passante per l'origine O , e perpendicolarmente a T sia definito un **asse di simmetria per rotazione** di ordine n (= il cristallo e' invariante per rotazioni di $2\pi/n$) (punti reticolari in blu)



$$2T \cos\left(\frac{2\pi}{n}\right) = Tm \quad m \in \mathfrak{S}$$

$\Rightarrow n = 1, 2, 3, 4, 6$ uniche simmetrie di rot. possibili

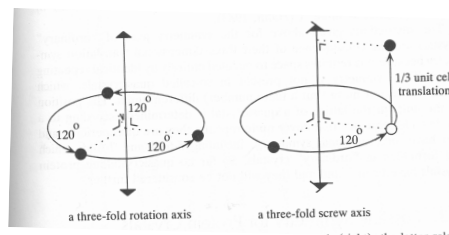
3

screw axis = roto-traslazione

Sia t la componente traslazionale di uno "**screw axis**", se l'asse di rotazione   di ordine n si deve avere:

$$nt = Tm \quad \text{con} \quad m \in \mathfrak{S}$$

$$\text{e dunque} \quad t = T \frac{m}{n}$$



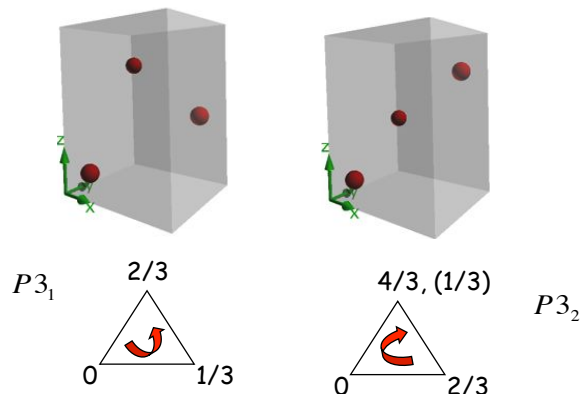
Il pi  piccolo valore possibile di m   1, e comunque si deve avere: $t = T \frac{m}{n} \leq T$

se $n=2 \Rightarrow t=T/2$ Simbologia per indicare gli **screw axes**: $2_1 \Rightarrow n=2, m=1$

$$n=3, m=1 \text{ o } m=2 \quad t = T \frac{m}{n} = \begin{cases} T \frac{1}{3} \Rightarrow 3_1 & \text{Per ogni rotazione di } 120^\circ \text{ si ha una traslazione di } 1/3 \\ & \text{del vettore di cella elementare } (3_1) \\ T \frac{2}{3} \Rightarrow 3_2 & \text{Per ogni rotazione di } 120^\circ \text{ si ha una traslazione di } 2/3 \\ & \text{del vettore di cella elementare } (3_2) \end{cases}$$

4

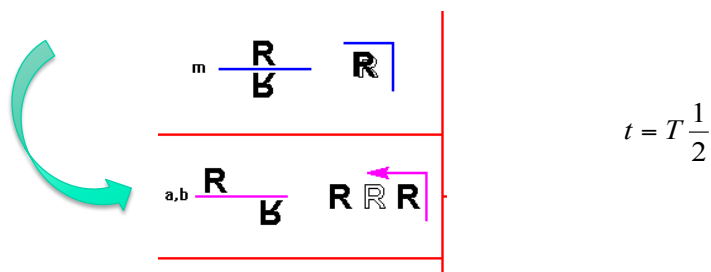
Se si uniscono gli oggetti generati dalla simmetria 3_1 si ottiene un **elica destrorsa**;
 Se si uniscono gli oggetti generati dalla simmetria 3_2 si ottiene un **elica sinistrorsa**;
 Le due eliche sono **enantiomorfe**



possibili screw axes:

$n=2, 2_1; n=3, 3_1, 3_2; n=4, 4_1, 4_2, 4_3; n=6, 6_1, 6_2, 6_3, 6_4, 6_5$

Glide plane = piano di scorrimento: riflessione + traslazione



5

Simmetrie e gruppi puntuali

<http://www.reciprocalnet.org/edumodules/symmetry/intro.html>

Operatori di simmetria:

E - operatore identità

σ - riflessione rispetto ad un piano

C_n - rotazione attorno ad un asse di $2\pi/n$

S_n - rotazione seguita da riflessione rispetto ad un piano \perp all'asse di rot. (**rotazione impropria**)

i - inversione rispetto ad un punto ($=S_2$)

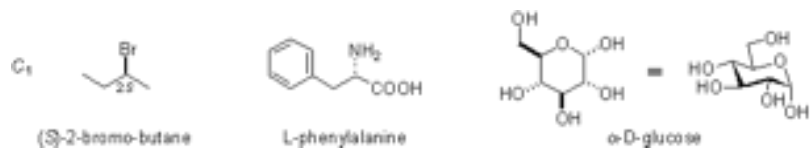
Ad un oggetto tridimensionale e' possibile associare un **gruppo** di simmetria; un **gruppo** gode delle seguenti proprietà:

1. deve contenere un operatore identità
2. il prodotto di due operatori deve appartenere al gruppo
3. il prodotto e' associativo: $A(BC)=(AB)C$
4. deve esistere un operatore inverso per ogni operatore

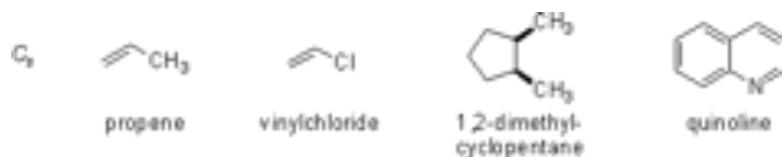
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Gruppi puntuali (notazione di Schönflies)

C_1 - assenza di qualsiasi simmetria



C_s - piano di riflessione



C_i - centro di inversione



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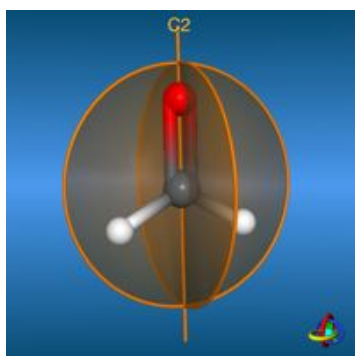
Gruppi puntuali (notazione di Schönflies)

C_n - asse di rotazione di ordine n ($2\pi/n$)



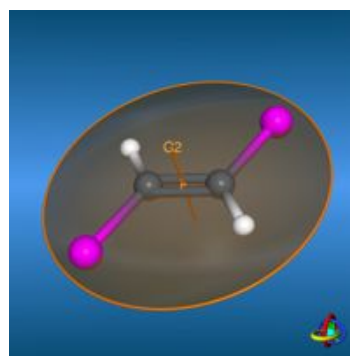
C_3

H_2CO
formaldeide, C_{2v}



C_{nv} - asse di rot. di ordine n + piano di riflessione verticale ($//$ all'asse di rot.) (σ_v)

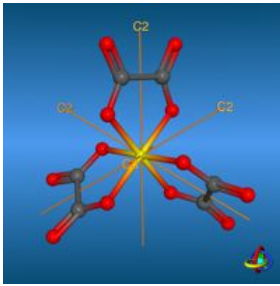
C_{nh} - asse di rot. di ordine n + piano di riflessione orizzontale (\perp all'asse di rot.) (σ_h)



dicloroetene, C_{2h}

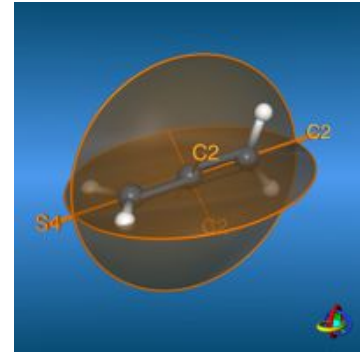
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D_3



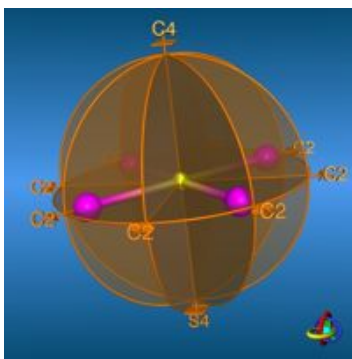
D_n - asse di rot. di ordine n (C_n) + n assi di rot. di ordine 2 (C_2) \perp (all'asse di ord. n)

D_{nd} - D_n + piano di riflessione diedrico (σ_d) collineare con l'asse principale e bisecante gli assi di rotazione C_2



D_{2d}

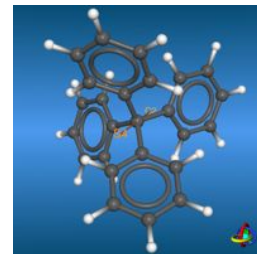
D_{4h}



D_{nh} - D_n + piano di riflessione orizzontale (\perp all'asse princ.) (σ_h)

9

S_n - rot. di ordine n seguita da riflessione rispetto ad un piano \perp all'asse di rot. (rot. impropria)

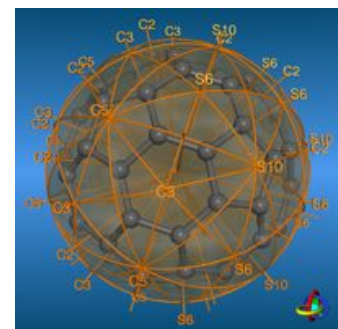


S_4

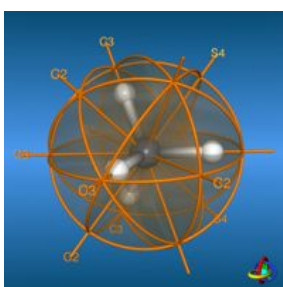
Gruppi puntuali speciali

- $D_{\infty h}$ - mol. biatomiche omonucleari
- $C_{\infty v}$ - mol. biatomiche eteronucleari
- T_d T_h - tetraedrico
- O_h - ottaedrico
- I_h - icosaedro
- K_h - sfera

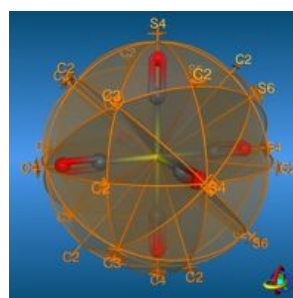
I_h



T_d

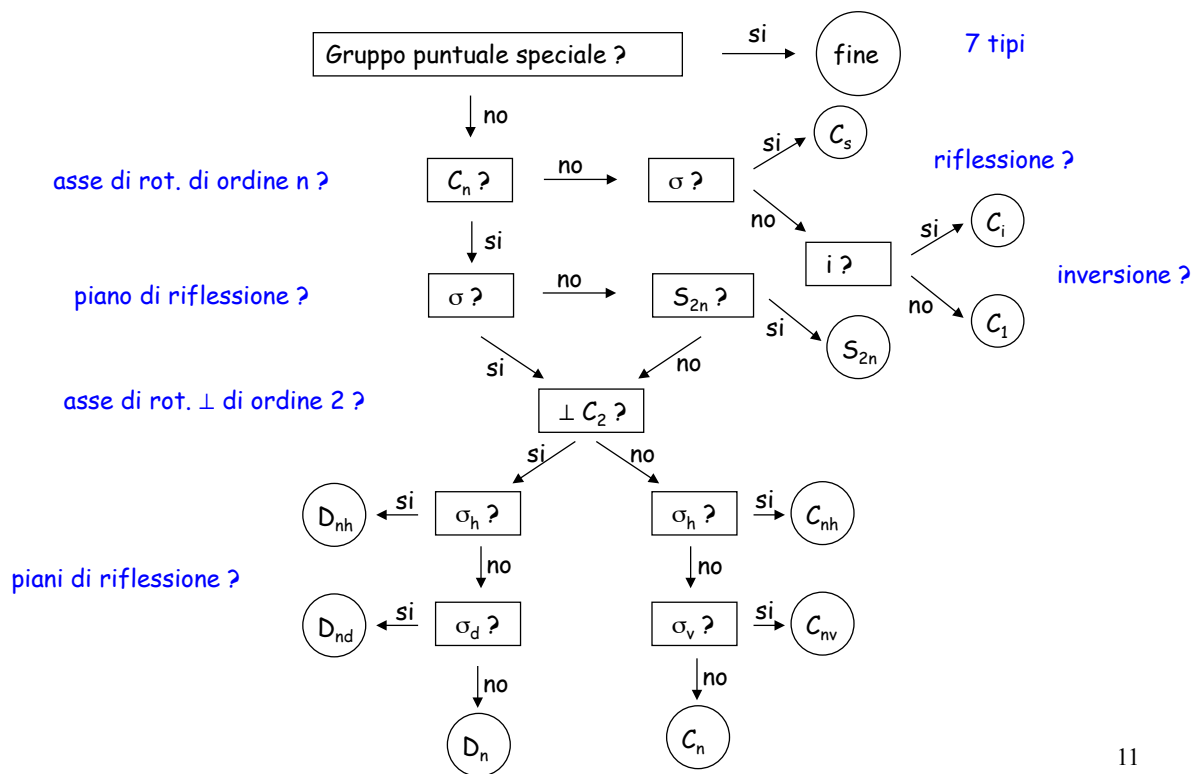


O_h

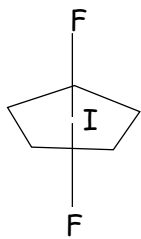


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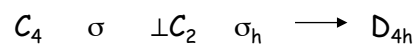
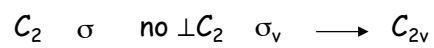
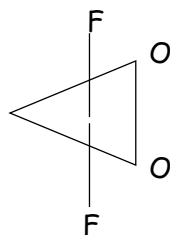
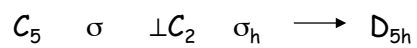
Riconoscimento del gruppo puntuale (17 tipi diversi)



11



Esempi



12

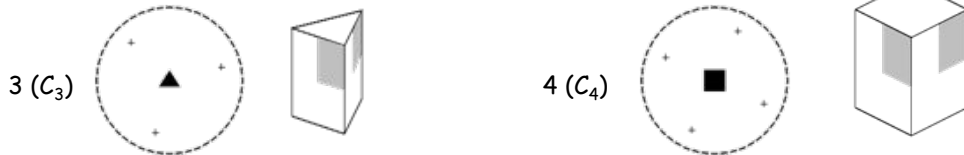
Asi propri: congruenza diretta, stessi angoli nei 2 oggetti legati da simmetria (rotazione)

Asi impropri: congruenza inversa, angoli opposti nei 2 oggetti legati da simmetria (rotazione + riflessione)

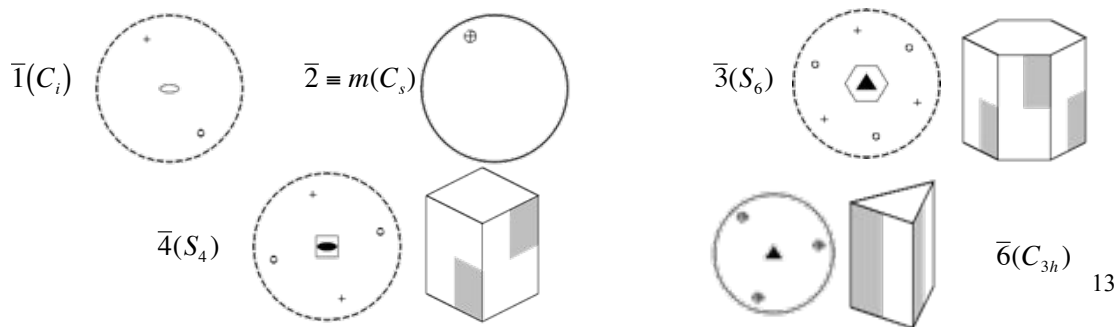
Point group = gruppi puntuali: combinazione di operatori che *non implicano traslazione*

Nello spazio tridimensionale del cristallo ci possono essere solamente **32 gruppi puntuali:**
 ("1" notazione internazionale, (C_i) notazione di Schoenflies)

5 assi propri (assi di rotazione): 1 (C_1), 2 (C_2), 3 (C_3), 4 (C_4), 6 (C_6)



5 assi impropri (rotazione + riflessione): $\bar{1}(C_i)$, $\bar{2} \equiv m(C_s)$, $\bar{3}(S_6)$, $\bar{4}(S_4)$, $\bar{6}(C_{3h})$



3 assi proprio + improprio: $2/\bar{2} \equiv 2/m(C_{2h})$, $4/m(C_{4h})$, $6/m(C_{6h})$



32 gruppi puntuali:

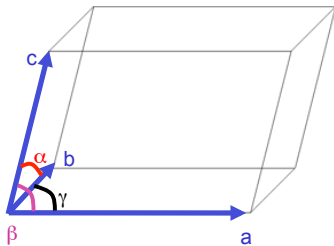
simmetria crescente

7 Crystal System	Unit Cell Parameters	32 Point Groups
Triclinic	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$	$C_1 C_i$
Monoclinic	$a \neq b \neq c; \alpha = \beta = 90^\circ \neq \gamma$	$C_2 C_2h$
Orthorhombic	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$	$C_2v D_2 D_{2h}$
Tetragonal	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$	$C_4 S_4 C_{4h} C_{4v} D_{2d} D_4 D_{4h}$
Trigonal	$a = b = c; \alpha = \beta = \gamma \neq 90^\circ$	$C_3 S_6 C_{3v} D_3 D_{3d}$
Hexagonal	$a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$	$C_3h C_6 C_{6h} C_{6v} D_{3h} D_6 D_{6h}$
Cubic	$a = b = c; \alpha = \beta = \gamma = 90^\circ$	$T T_h T_d O O_h$

Esistono **7 sistemi cristallini (crystal system):** triclino, monoclinico, ortorombico, trigonale, tetragonale, esagonale, cubico

Esistono **230 gruppi spaziali cristallografici:** <http://img.chem.ucl.ac.uk/sgp/large/sgp.htm>

Crystal Systems Defined in Terms of Minimal Symmetry

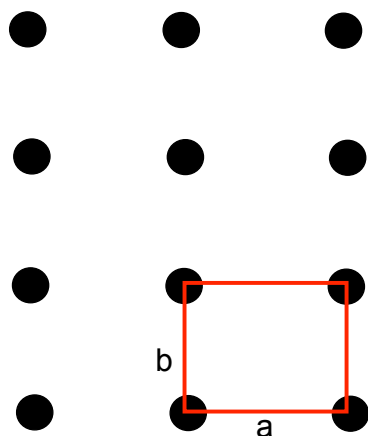


System	Minimal Symmetry	Cell Conditions
Triclinic	No Symmetry	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2-fold (along b)	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$
Orthorhombic	3 perpendicular 2 folds	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	4-fold (along c)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Rhombohedral	3-fold along diagonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$
Hexagonal	6-fold (along c)	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$
Cubic	3-fold along all diagonals	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

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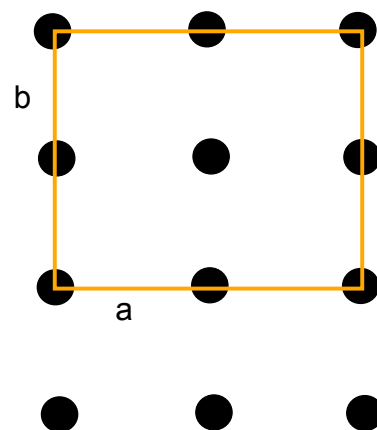
Lattice Types

What is convention for choosing cell?



Primitive Cell

- 1) Contains 1 lattice point
- 2) Contains smallest possible volume

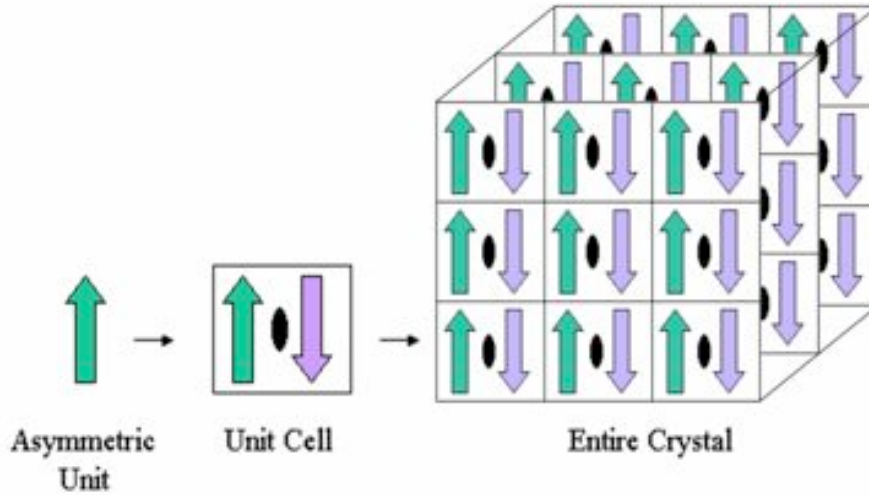


Centered Cell

- 1) Contains multiple lattice points
- 2) Contains integral multiple of primitive volume

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Unita' asimmetrica



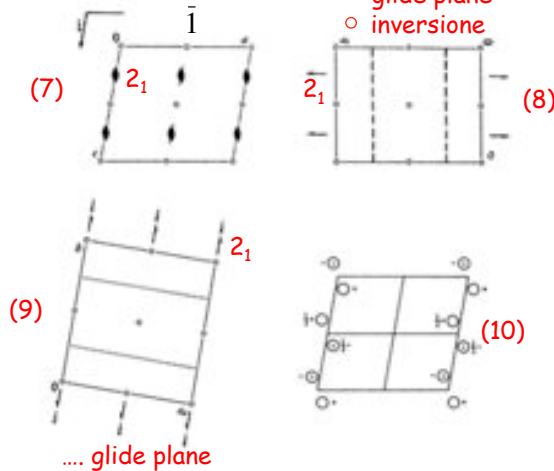
http://cci.lbl.gov/asu_gallery/

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Tavole cristallografiche

- (1) $P2_1/c$ (3) C_{2h}^2 (3a) (4) $2/m$ (5) Monoclinic
 (2) No. 14 (6) $P12_1/c1$ Patterson symmetry $P12_1/m1$

UNIQUE AXIS b , CELL CHOICE 1



Origin $a,1$
 Asymmetric unit $0 \leq x \leq 1/2, 0 \leq y \leq 1, 0 \leq z \leq 1$
 Symmetry operations
 (1) 1 (2) 2_1 (3) c (4) 2_1c

- (1) Simbolo di Hermann-Mauguin
- (2) Numero del gruppo sp. (1-230)
- (3) Simbolo di Schoenflies ((3a) apice: simbolo del gruppo spaziale)
- (4) (gruppo puntuale **notazione internazionale**)
- (5) Sistema cristallografico
- (6) Simbolo di Hermann-Mauguin intero
- (7) Proiezione rispetto all'asse b
- (8) Proiezione rispetto ad a
- (9) Proiezione rispetto a c
- (10) Posizioni generali nella cella
- (11) Operazioni di simmetria

(11)

inversione



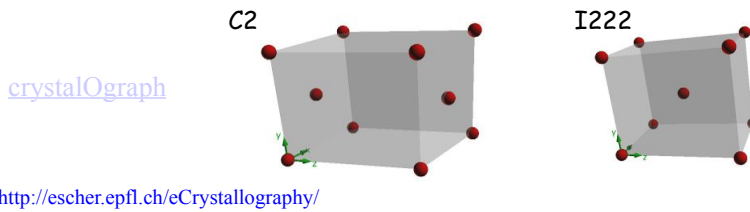
18

230 gruppi spaziali $\xrightarrow[\text{chiralita'}]{\text{tolgo } C_i, C_s}$ diventano 65

65 gruppi spaziali per mol. enantiomorfe (Proteine)

- Triclino P1 (1)
- Monoclino P2, P2₁, C2 (3)
- Ortorombico F222, I222, I2₁2₁2₁, C222, C222₁, P222, P222₁, P2₁2₁2, P2₁2₁2₁ (9)
- Tetragonale I4, I4₁, I422, I4₁22, P4, P4₁₋₃, P422, P42₁2, P4₁₋₃22, P4₁₋₃2₁2 (16)
- Esagonale P3, P3₁₋₂, P312, P3₁₋₂12, P321, P3₁₋₂21, P6, P6₁₋₅, P622, P6₁₋₅22 (21)
- Trigonale R3, R32 (2)
- Cubico P23, P2₁3, P432, P4₁₋₃32, I23, I2₁3, I432, I4₁32, F23, F432, F4₁32 (13)

P = cella primitiva (1 punto reticolare per cella, coord. (0,0,0))
 C = cella centrata nella faccia C (2 punti reticolari per cella, coord. (0,0,0), (0.5, 0.5,0))
 F = cella centrata su tutte le facce (4 punti reticolari per cella)
 I = cella centrata al centro (2 punti reticolari per cella, coord. (0,0,0), (0.5, 0.5,0.5))
 R = cella primitiva



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P2₁ **C₂²** 2 **Monoclini**
 No. 4 P12₁1 Patterson symmetry P12/n

UNIQUE AXIS *b*
 $\beta \neq 90^\circ$

2 unità asimmetriche
 $x, y, z \quad \bar{x}, y + \frac{1}{2}, \bar{z}$
 a b

Origin on 2,
 Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq \frac{1}{2}$
 Symmetry operations
 (1) 1 (2) 2(0, 1/2, 0) 0, y, 0

Monoclino $a \neq b \neq c; \alpha = \gamma = 90^\circ \neq \beta \quad C_2$

20

$P222$

No. 16

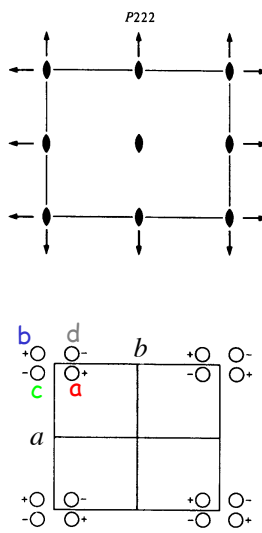
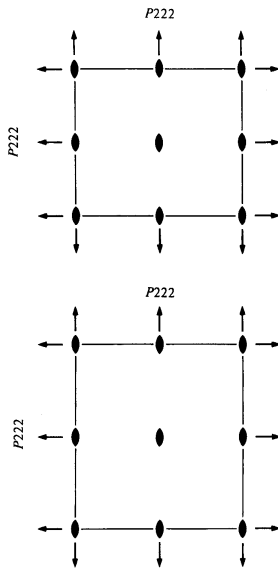
D_2^1

$P222$

222

Ortho

Patterson symm



4 unità asimmetriche

x, y, z \bar{x}, \bar{y}, z
 a b
 \bar{x}, y, \bar{z} x, \bar{y}, \bar{z}
 c d

Origin at 222

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

Symmetry operations

- (1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

Ortorombico $a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ D_{2h}$

21

$C222_1$

No. 20

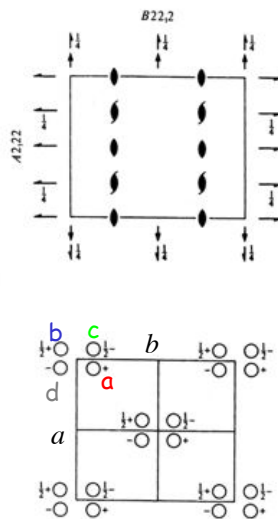
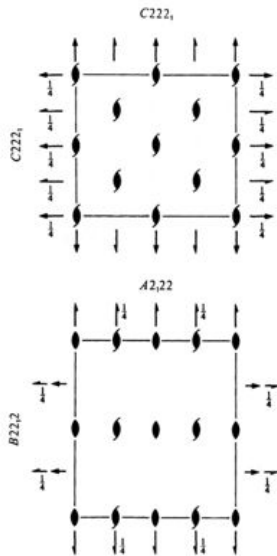
D_2^5

$C222_1$

222

Orthorh

Patterson symmetry



8 unità asimmetriche

$0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, 0$
 x, y, z $\bar{x}, \bar{y}, z + \frac{1}{2}$
 a b
 $\bar{x}, y, \bar{z} + \frac{1}{2}$ x, \bar{y}, \bar{z}
 c d

Origin at 212

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

Symmetry operations

For $(0,0,0)+$ set

- (1) 1 (2) 2 $(0,0,\frac{1}{2})$ $0,0,z$ (3) 2 $0,y,\frac{1}{2}$ (4) 2 $x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- (1) $i(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $(0,0,\frac{1}{2})$ $\frac{1}{2},\frac{1}{2},z$ (3) 2 $(0,\frac{1}{2},0)$ $\frac{1}{2},y,\frac{1}{2}$ (4) 2 $(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$

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$I4_122$

D_4^{10}

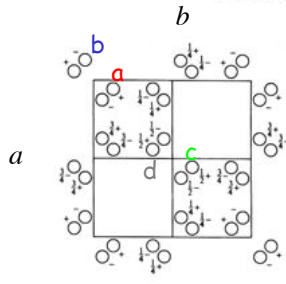
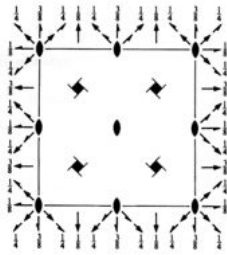
422

Tetra

No. 98

$I4_122$

Patterson symmetry I



16 unità asimmetriche

$0, 0, 0 \quad \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

$x, y, z \quad \bar{x}, \bar{y}, \bar{z}$

$x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$

$\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$

d

(...)

Origin at 222 at 212

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

Symmetry operations

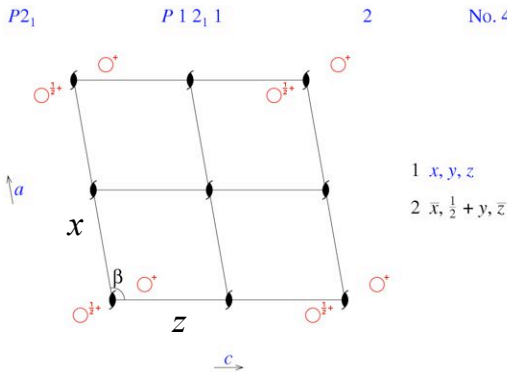
For (0,0,0)+ set

- (1) 1
- (2) $2(0,0,\frac{1}{2}) \parallel z$
- (3) $4^+(0,0,\frac{1}{2}) \parallel z$
- (4) $4^-(0,0,\frac{1}{2}) \parallel z$
- (5) $2 \parallel x, \frac{1}{2}$
- (6) $2 \parallel x, \frac{1}{2}, \frac{1}{2}$
- (7) $2(\frac{1}{2}, \frac{1}{2}, 0) \parallel x, x, \frac{1}{2}$
- (8) $2 \parallel x, \bar{x}, 0$

For (1,1,1)+ set

- (1) $i(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- (2) $2 \parallel 0,0,z$
- (3) $4^+(0,0,\frac{1}{2}) \parallel z$
- (4) $4^-(0,0,\frac{1}{2}) \parallel z$
- (5) $2(0,\frac{1}{2},0) \parallel 0,y,\frac{1}{2}$
- (6) $2(\frac{1}{2},0,0) \parallel x,0,\frac{1}{2}$
- (7) $2 \parallel x,x,0$
- (8) $2 \parallel x,\bar{x} + \frac{1}{2}, \frac{1}{2}$

Assenze sistematiche



$2_1 \Rightarrow \rho(x,y,z) = \rho(-x, y + \frac{1}{2}, -z)$

$F(h,k,l) = \int_{cell} \rho(x,y,z) \exp[2\pi i(hx + ky + lz)] dV$

F.t.

$\rho(x,y,z) = \frac{1}{V} \sum_{h,k,l} F(h,k,l) \exp[-2\pi i(hx + ky + lz)]$

Translational Symmetry Elements and Their Extinctions

Symmetry element	Affected reflection	Condition for systematic absence of reflection
2-fold screw (2_1)	$h00$	$k = 2n + 1 = \text{odd}$
4-fold screw (4_1) along b	$0k0$	$k = 2n + 1$
6-fold screw (6_1) along c	$00l$	$l = 2n + 1$
3-fold screw ($3_1, 3_2$)	$*c$	$l = 3n + 1, 3n + 2$
6-fold screw ($6_2, 6_4$) along a	$h00$	$h = 4n + 1, 2, \text{ or } 3$
4-fold screw ($4_2, 4_3$) along b	$0k0$	$k = 4n + 1, 2, \text{ or } 3$
6-fold screw ($6_3, 6_5$) along c	$00l$	$l = 4n + 1, 2, \text{ or } 3$
6-fold screw (6_6) along $*c$	$*c$	$l = 6n + 1, 2, 3, 4, \text{ or } 5$
Glide plane perpendicular to translation $b/2$ (b glide)	$0kl$	$k = 2n + 1$
$c/2$ (c glide)		$l = 2n + 1$
$b/2 + c/2$ (nc glide)		$k + l = 2n + 1$
$b/4 + c/4$ (d glide)		$k + l = 4n + 1, 2, \text{ or } 3$
Glide plane perpendicular to translation $a/2$ (a glide)	$h0l$	$h = 2n + 1$
$c/2$ (c glide)		$l = 2n + 1$
$a/2 + c/2$ (nc glide)		$h + l = 2n + 1$
$a/4 + c/4$ (d glide)		$h + l = 4n + 1, 2, \text{ or } 3$
Glide plane perpendicular to translation $a/2$ (a glide)	hkl	$h = 2n + 1$
$b/2$ (b glide)		$k = 2n + 1$
$a/2 + b/2$ (nc glide)		$h + k = 2n + 1$
$a/4 + b/4$ (d glide)		$h + k = 4n + 1, 2, \text{ or } 3$
A-centered lattice (A)	hkl	$k + l = 2n + 1$
B-centered lattice (B)		$h + l = 2n + 1$
C-centered lattice (C)		$h + k = 2n + 1$
Face-centered lattice (F)		$h + k = 2n + 1$ i.e., h, k, l not all even or all odd
		$h + l = 2n + 1$ all even or all odd
		$k + l = 2n + 1$ odd
Body-centered lattice (I)		$h + k + l = 2n + 1$

* Note that in the crystal classes in which 3- and 6-fold screws occur as cell axes, these are conventionally assigned to be c , so only the $00l$ reflections need be considered.

Assenze sistematiche

$$2_1 \Rightarrow (x, y, z) = (-x, y + \frac{1}{2}, -z)$$

$$F(h, k, l) = \int_{cell} \rho(x, y, z) \exp[2\pi i(hx + ky + lz)] dV$$

$$F(h, k, l) = \sum_j^{N/2} f_j \left\{ \exp[2\pi i(hx_j + ky_j + lz_j)] + \exp[2\pi i(-hx_j + k(y_j + 1/2) - lz_j)] \right\}$$

unita' asimmetriche

quando $h=0$ e $l=0$:

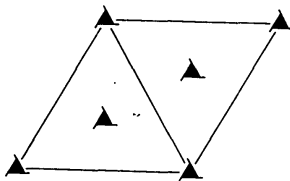
$$F(0, k, 0) = \sum_j f_j \exp[2\pi i(ky_j)] (1 + \exp(\pi i k))$$

$$|F(0, k, 0)|^2 \propto |1 + \exp(i\pi k)|^2 = 2(1 + \cos(\pi k)) = 0; \text{ se } k \text{ dispari}$$

25

$P3_1$

No. 144



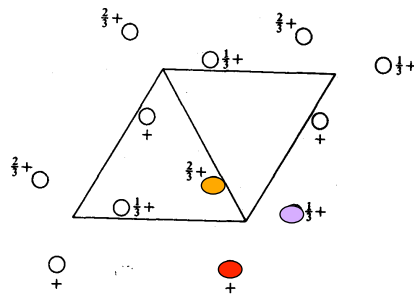
C_3^2

$P3_1$

3

Γ

Patterson sy1



agonal

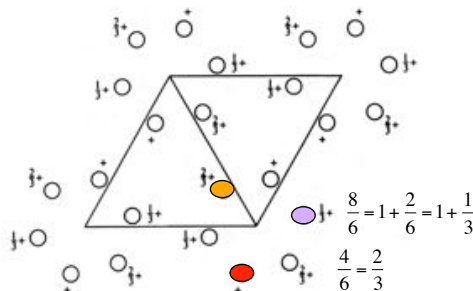
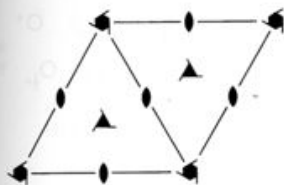
on symmetry $P6/m$

6

C_6^5

$P6_4$

N_3



Esempio: Bir3

26

pointless

mosflm: P3

Spacegroup		TotProb	SysAbsProb
<P 6 2 2>	(177)	0.714	0.606
<P 62 2 2>	(180)	0.408	0.347
<P 64 2 2>	(181)	0.408	0.347
<P 3>	(143)	0.022	0.606
<P 31>	(144)	0.012	0.347
<P 32>	(145)	0.012	0.347

P3	Low resolution limit	105.41	105.41	3.37
	High resolution limit	3.20	10.12	3.20
	Rmerge	0.086	0.037	0.335

P6	Low resolution limit	40.00	40.00	3.37
	High resolution limit	3.20	10.12	3.20
	Rmerge	0.093	0.038	0.362

P622	Low resolution limit	40.00	40.00	3.37
	High resolution limit	3.20	10.12	3.20
	Rmerge	0.176	0.084	0.432

P3

Phaser trova soluzione P3₁, 9 molecole ⇒ raffino e arrivo a 6 mol. ⇒ molrep 8 mol ⇒ reffmac R/Rfree = 29.2/35.9

P6

Phaser trova soluzione P6₄, 5 molecole ⇒ raffino e arrivo a 4 mol. ⇒ reffmac R/Rfree = 28.3/36.1

27

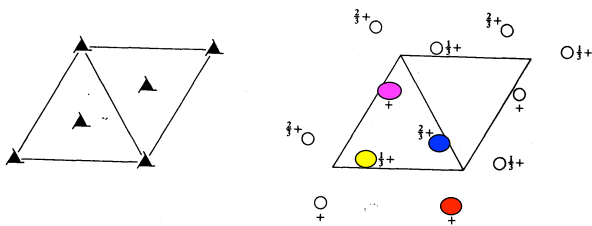
P3₁
No. 144

C₃²
P3₁

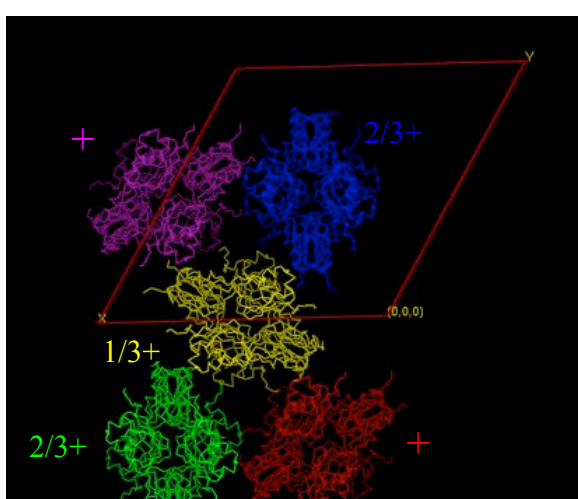
3

T

Patterson sy1



8 mol nell'u.a.



28

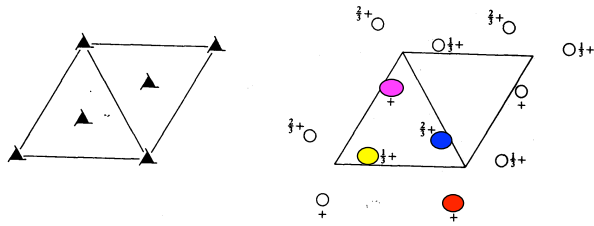
$P3_1$
No. 144

C_3^2
 $P3_1$

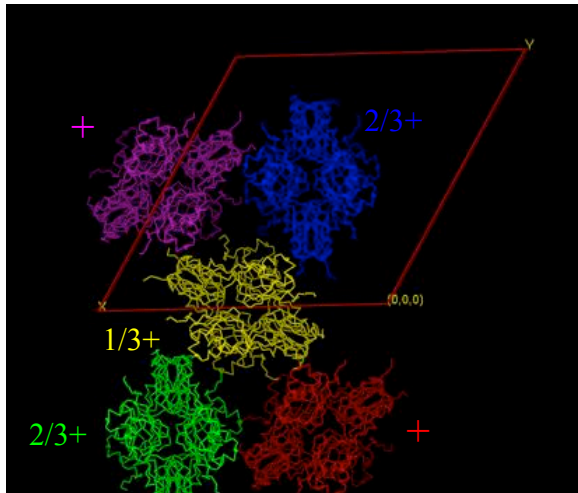
3

T

Patterson sy



8 mol nell'u.a.



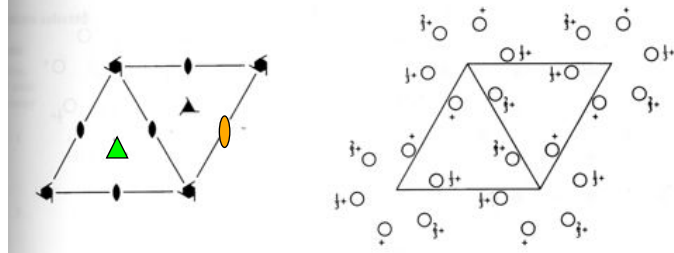
29

agonal
on symmetry $P6/m$

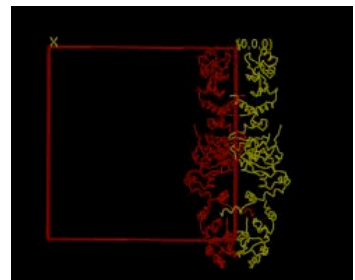
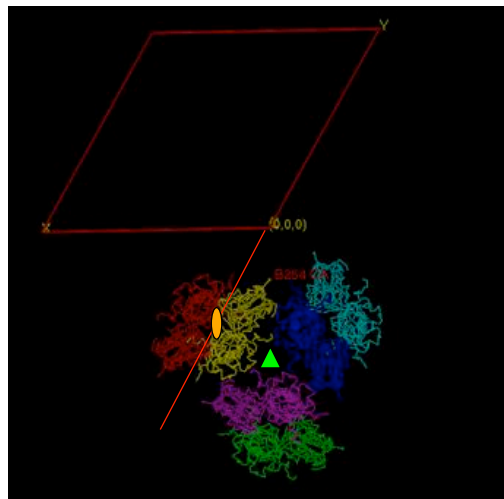
6

C_6^5
 $P6_4$

N

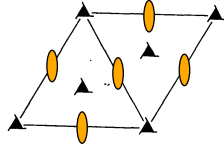


4 mol nell'u.a.



30

$P3_1 + \text{asse di ordine 2 in piu'} \Rightarrow P6_4$



\Rightarrow

