

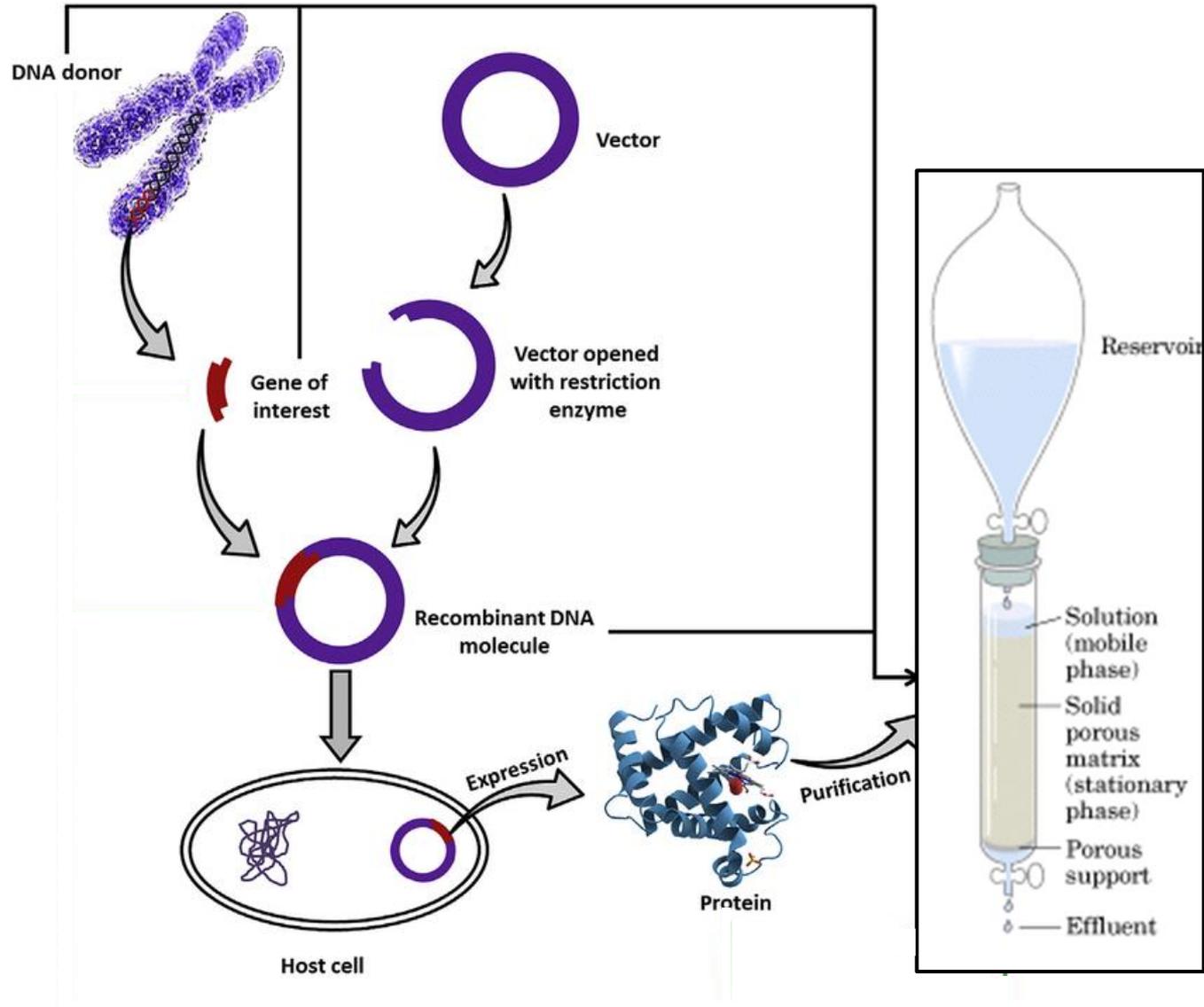
Cristais Protéicos e Simetria

Referências

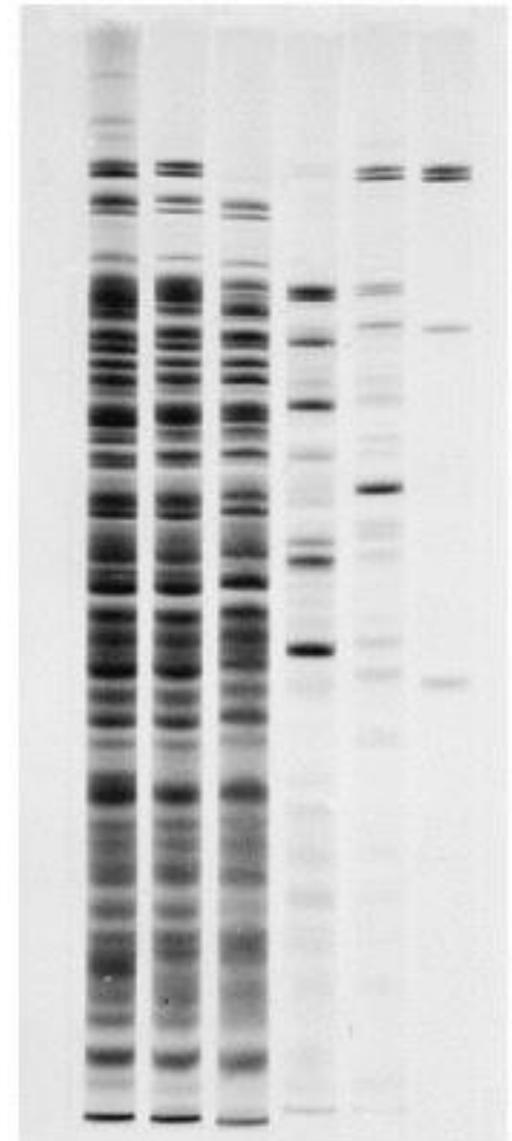
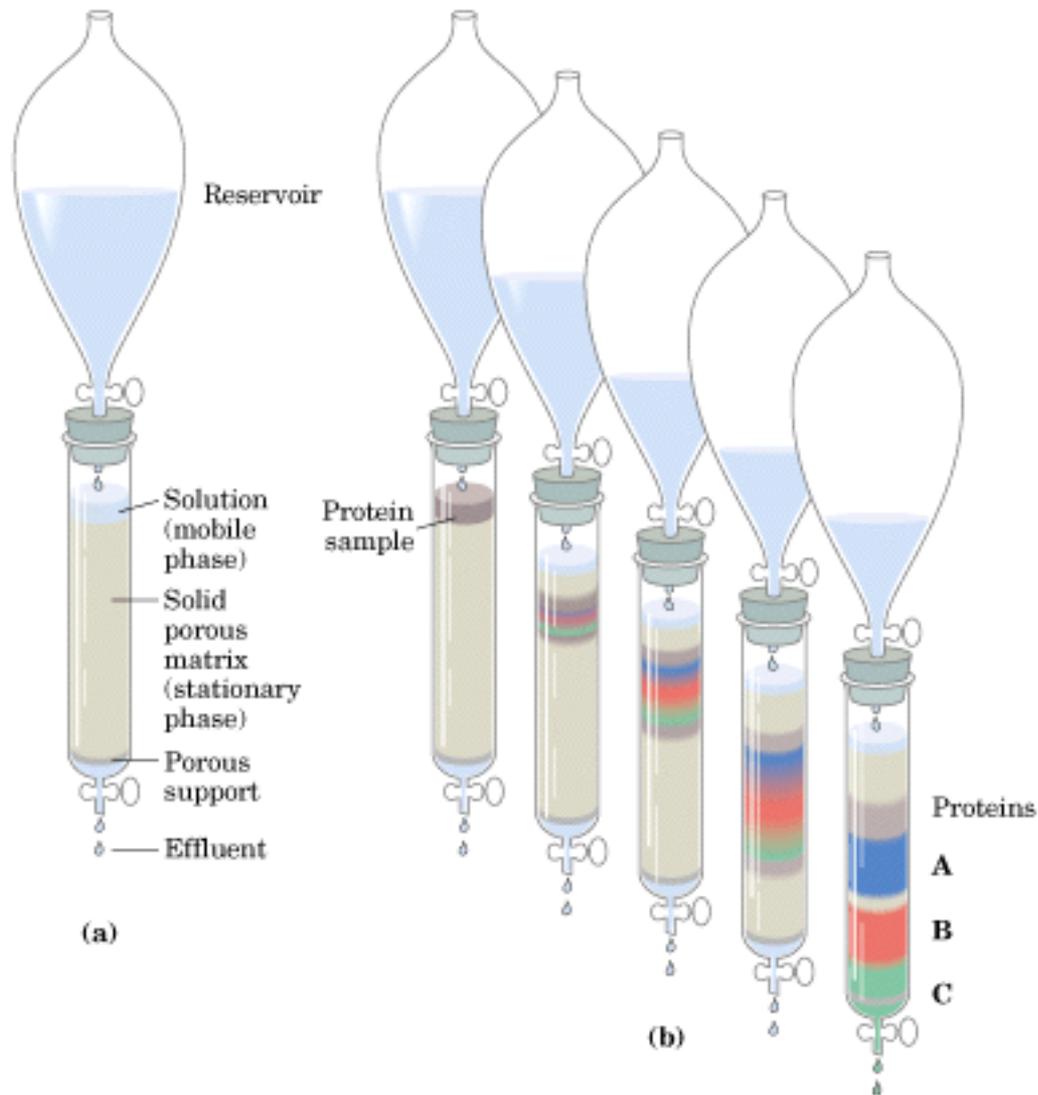
Gale Rhodes: Crystallography made
crystal clear (capítulos 2 e 3)

Jan Drenth: Principles of protein
X-ray crystallography (Capítulo 3)

Cristais Proteicos e Simetria

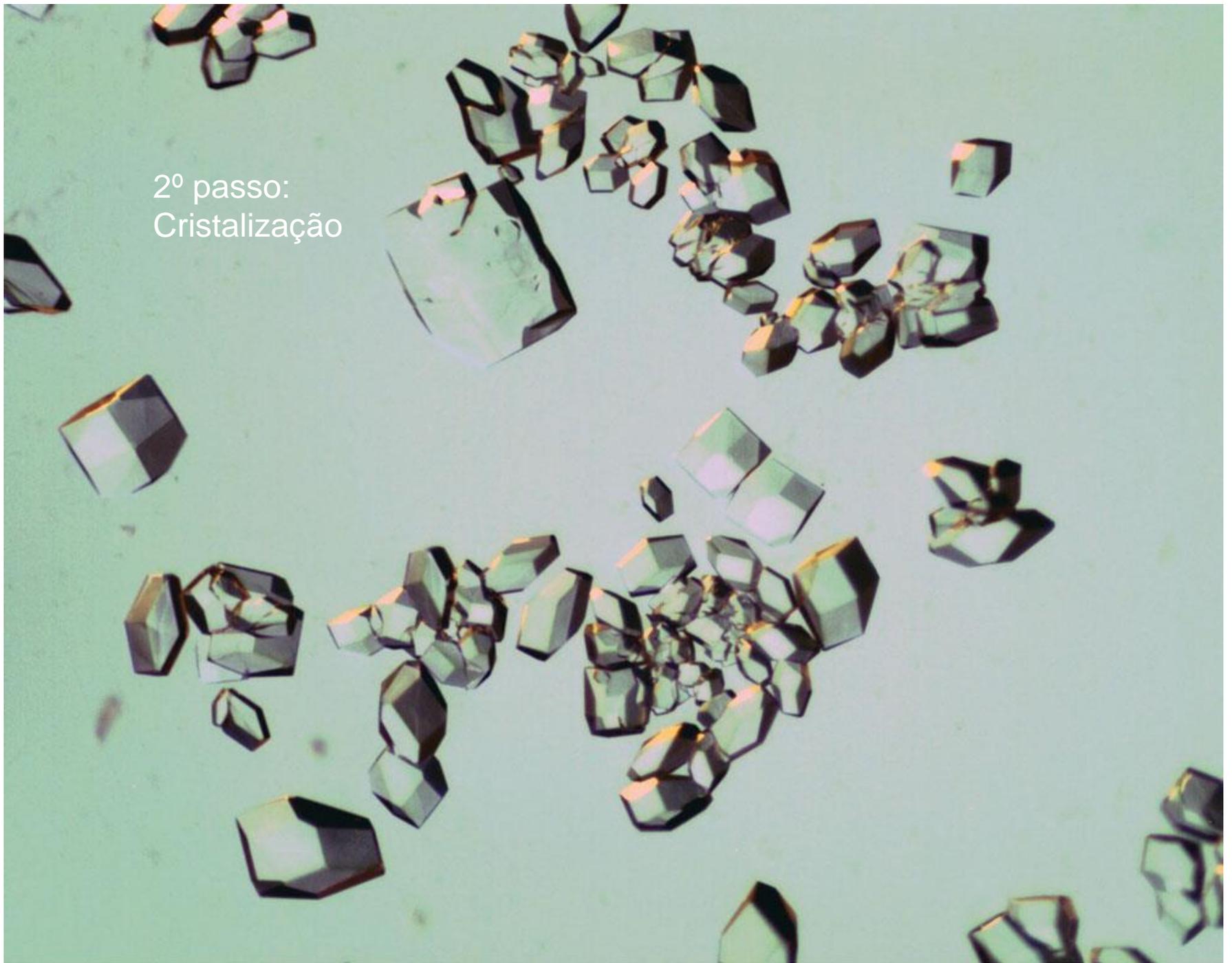


1º passo: Purificação da macromolécula de interesse

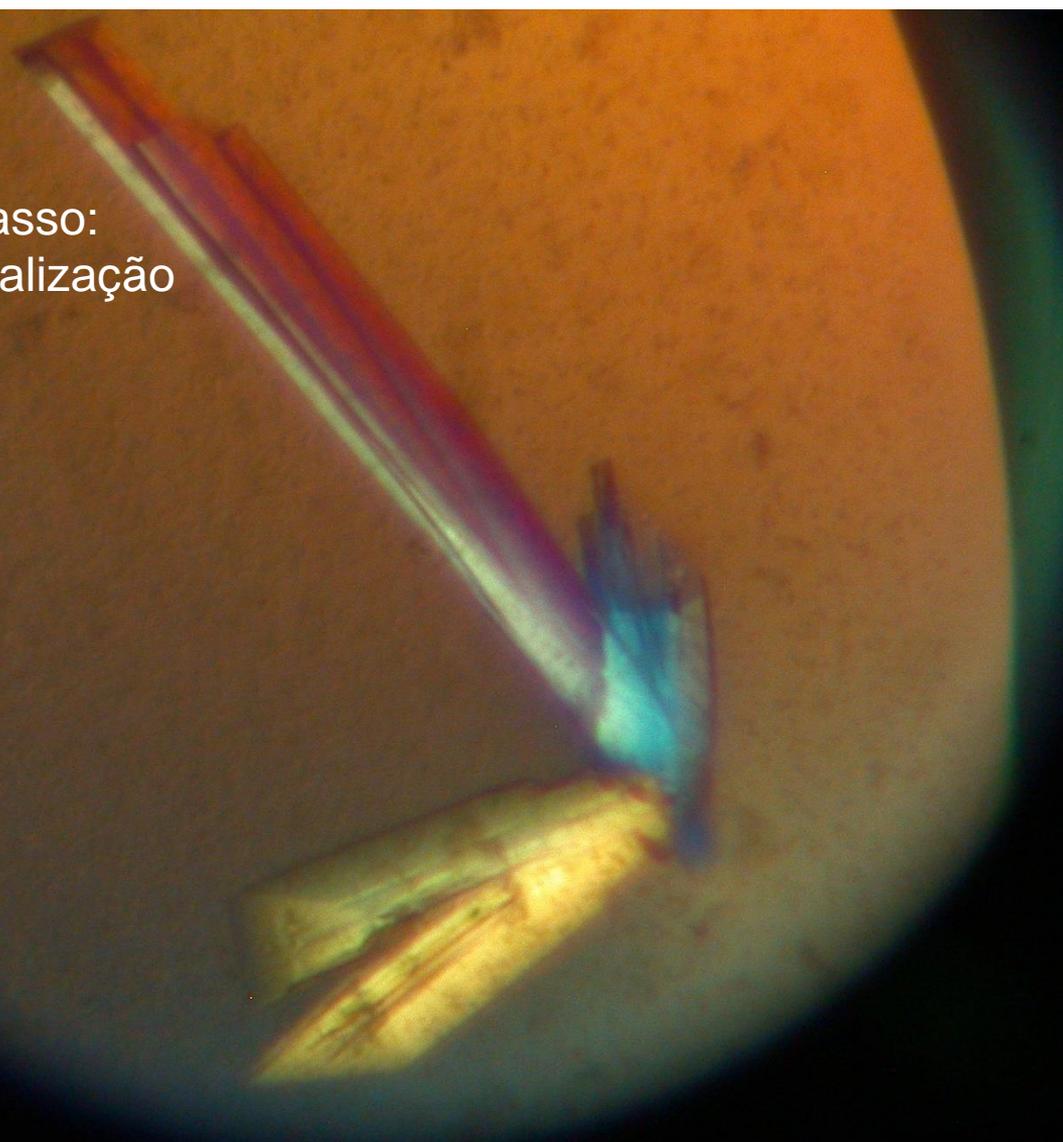




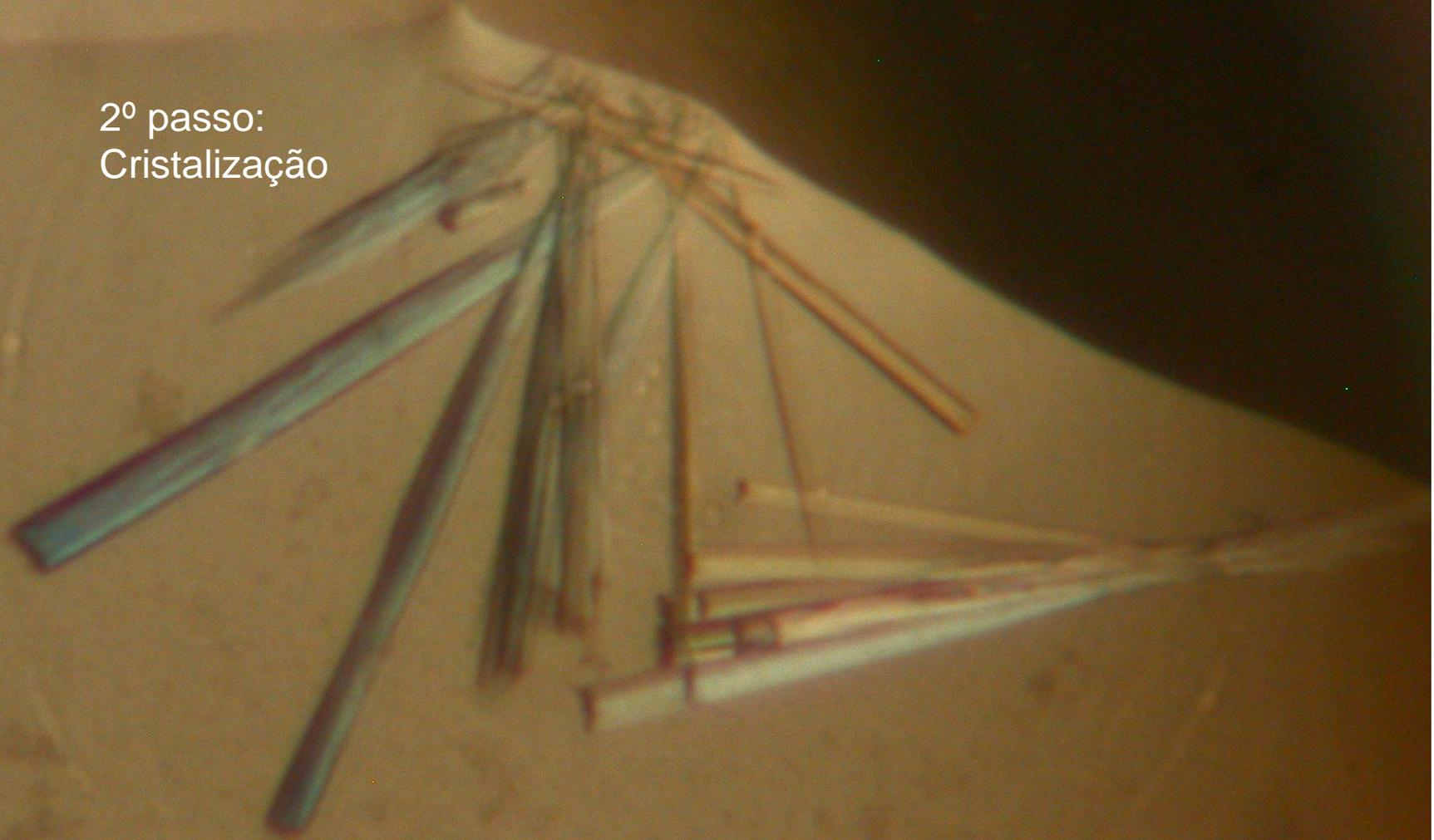
2º passo:
Cristalização



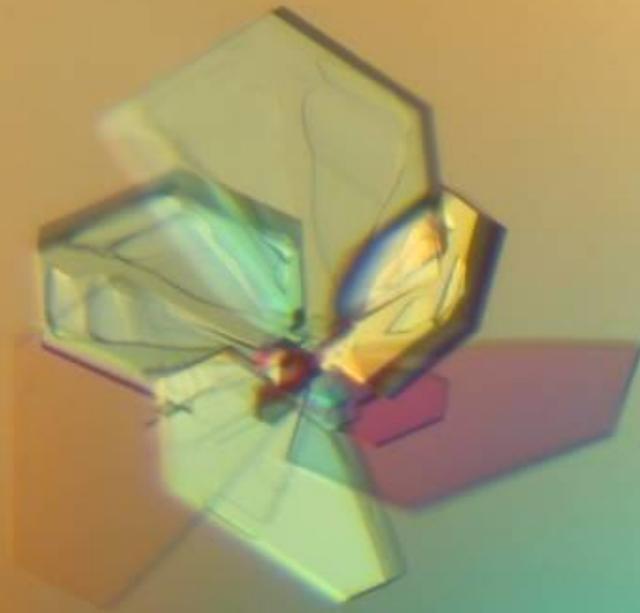
2º passo:
Cristalização

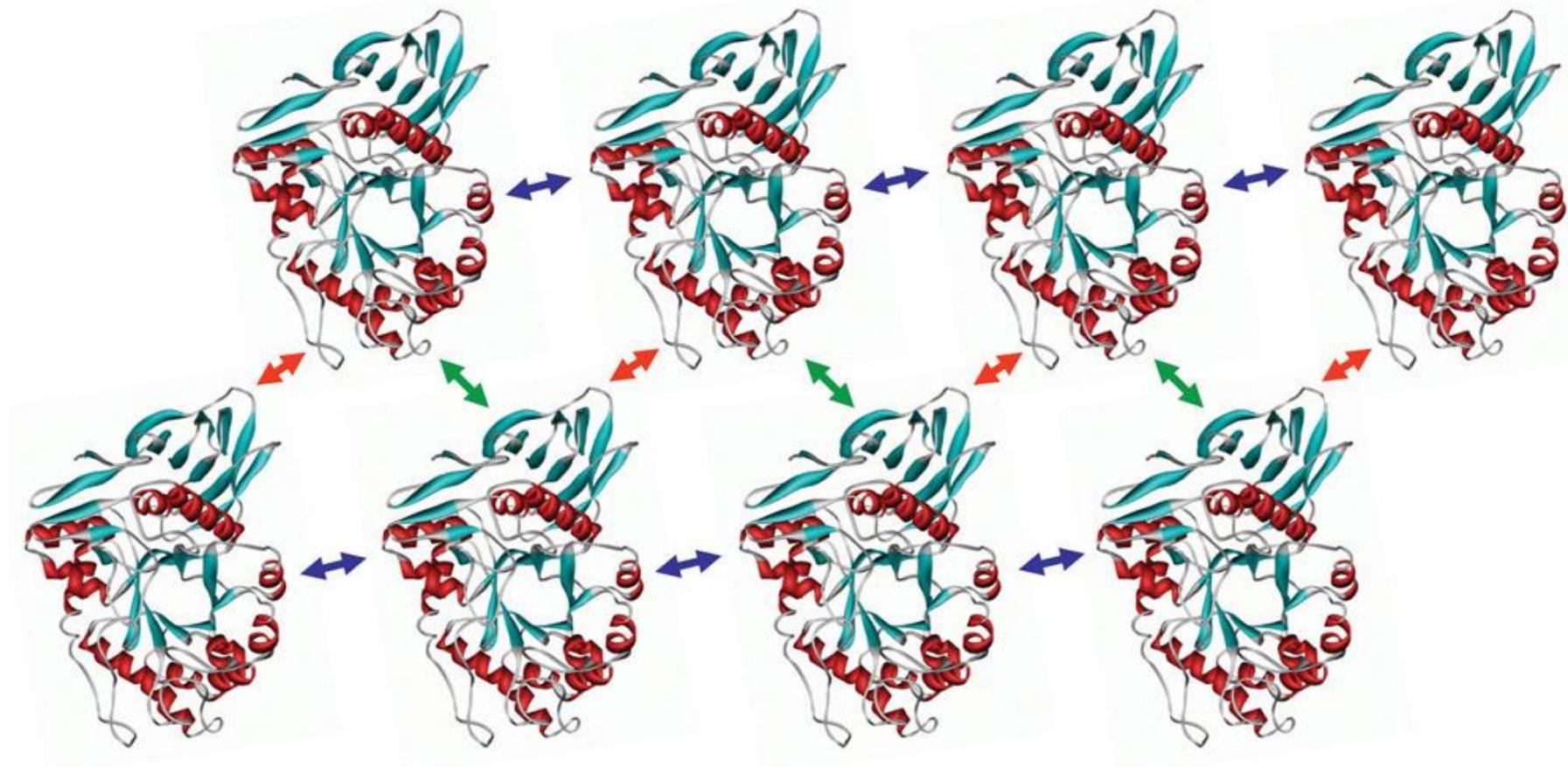


2º passo:
Cristalização



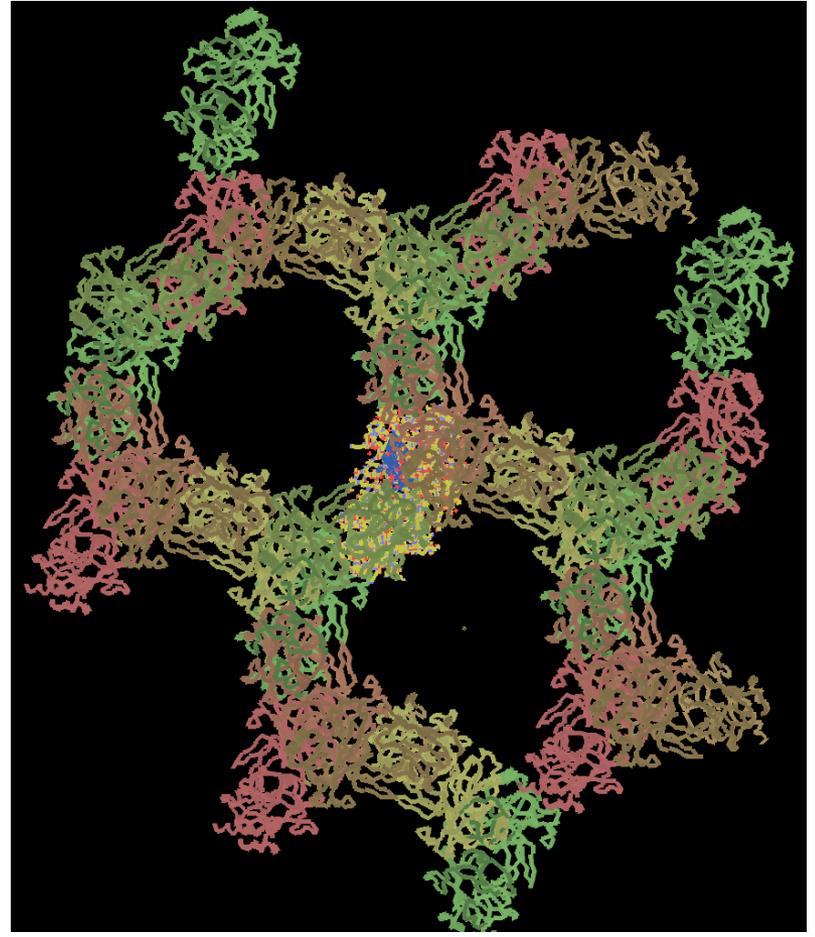
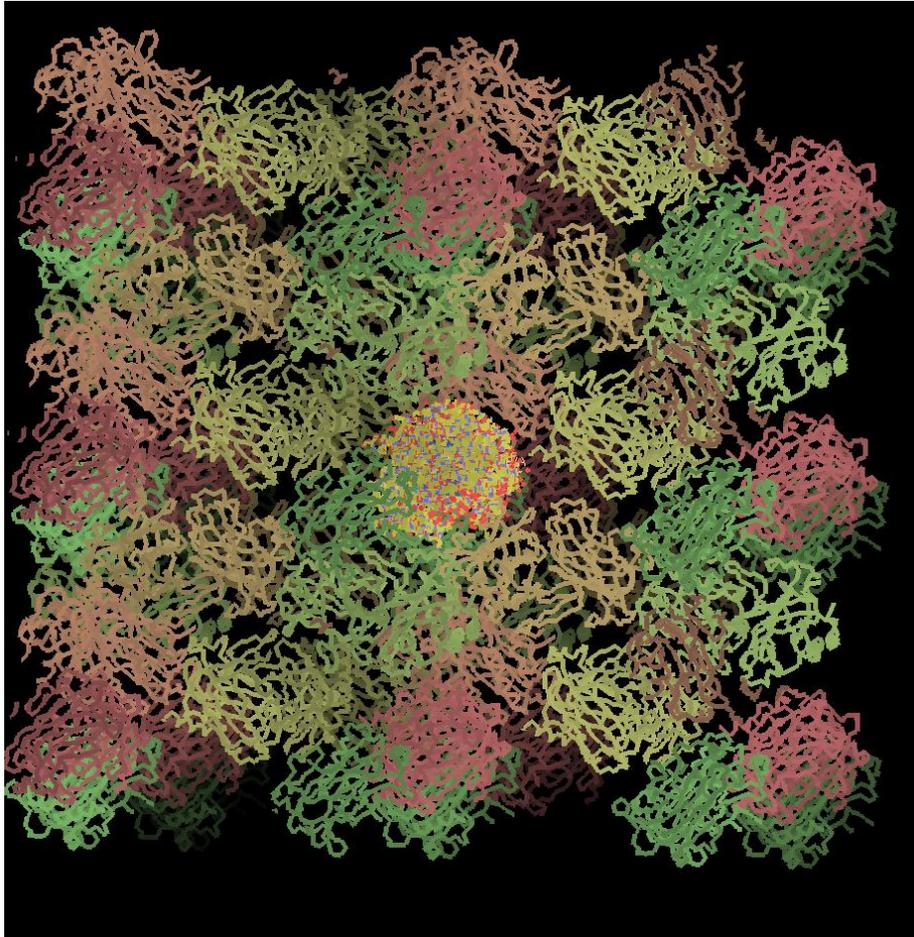
2º passo:
Cristalização

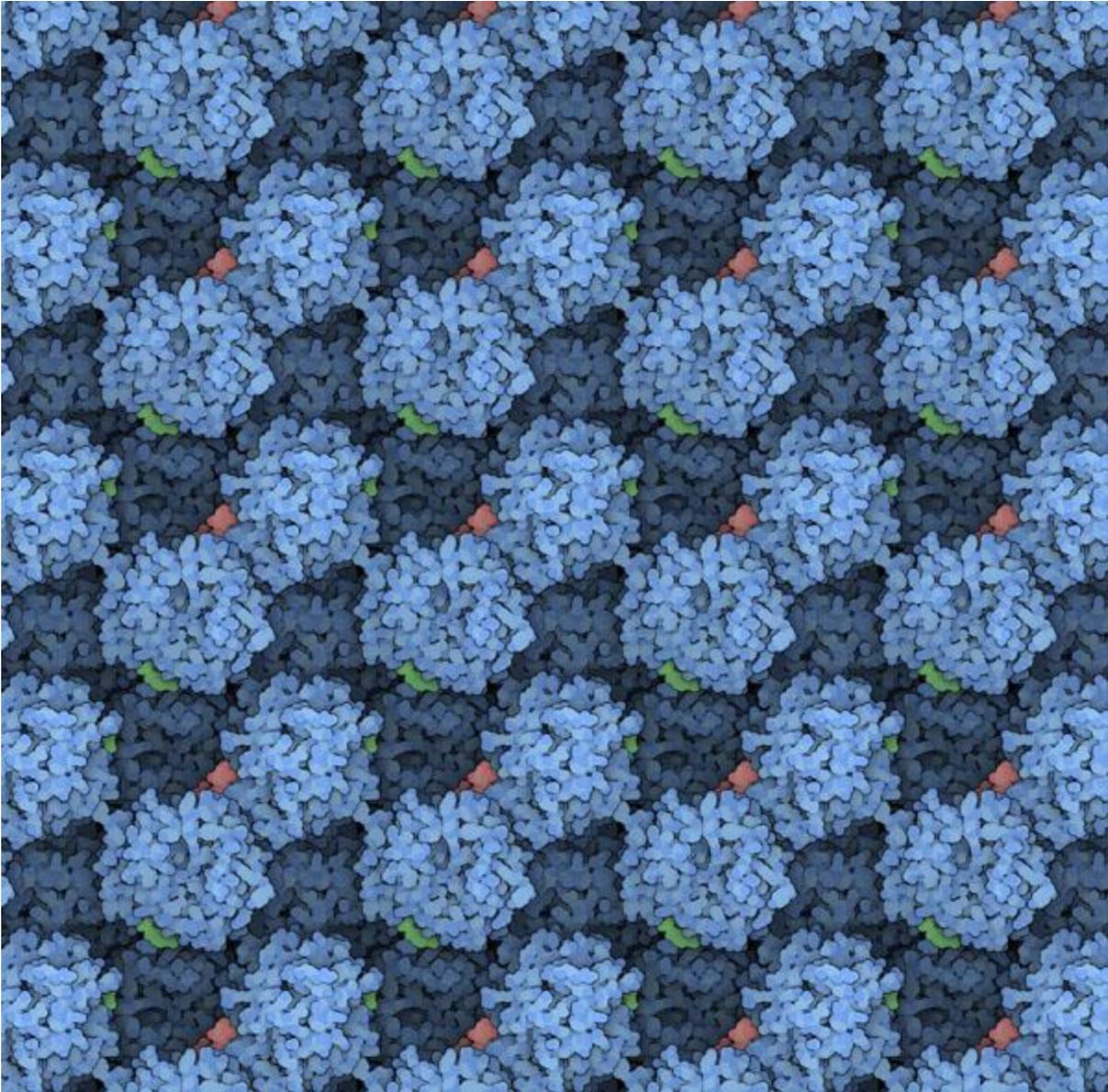




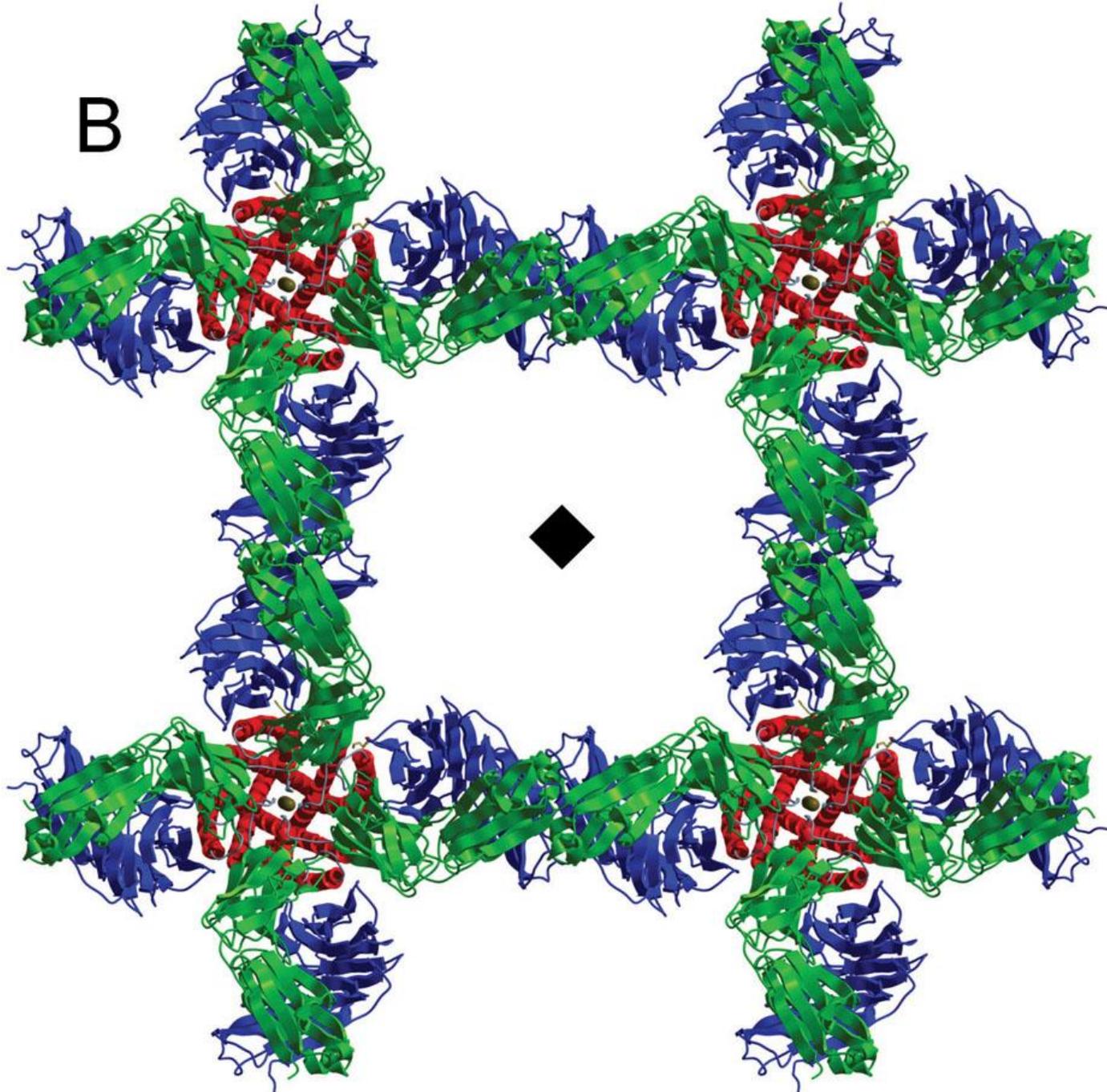
Forças relativamente fracas (ligações não-covalentes) entre moléculas dentro do cristal: pontes de hidrogênio, pontes salinas, interações van der Waals, efeito hidrofóbico

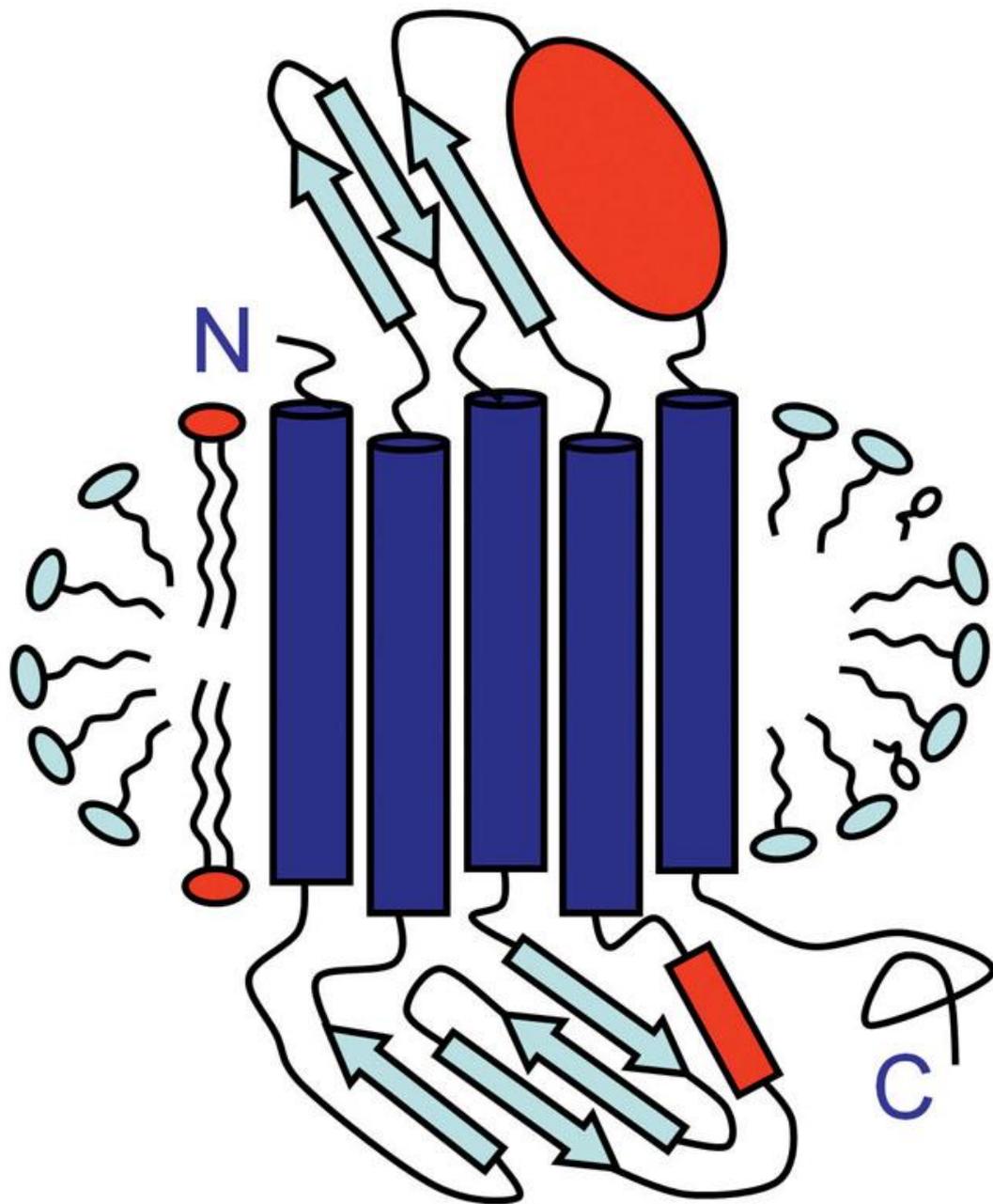
Crystals have from between 25 -75% water



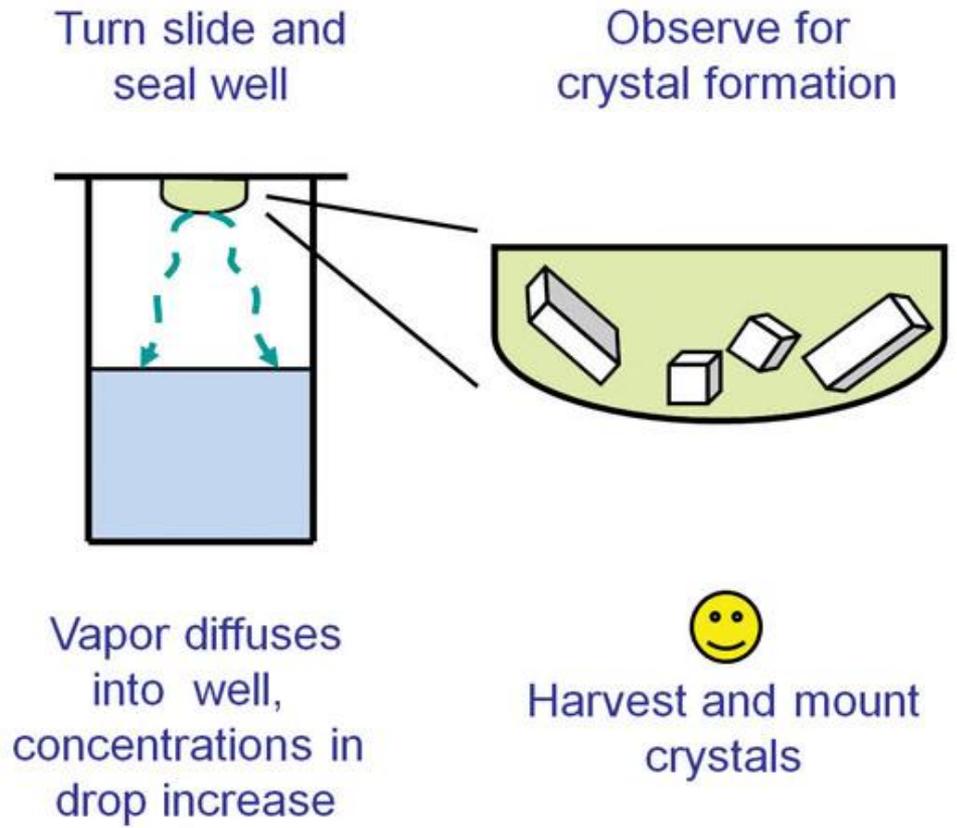
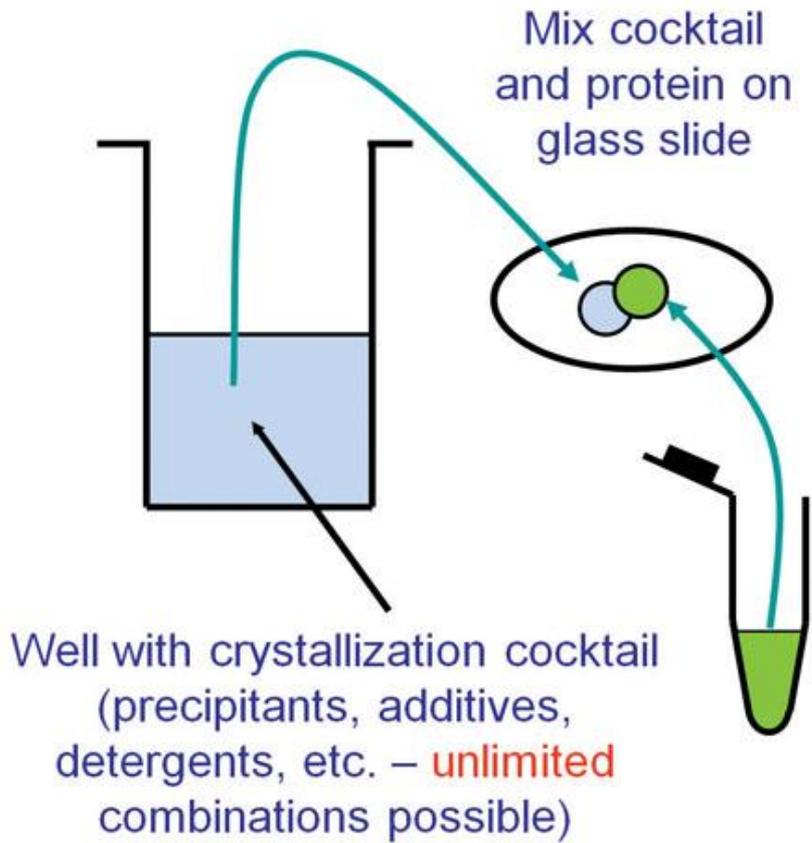


B



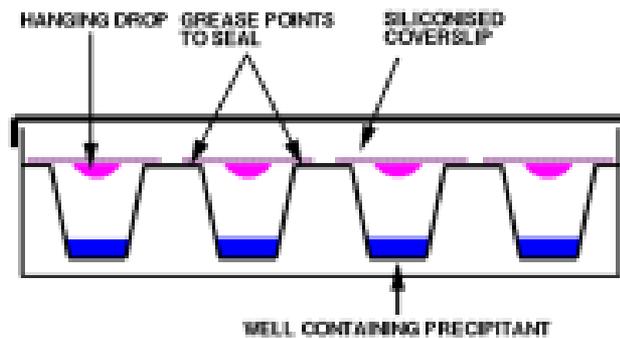


-  Membrane phospholipid
-  Detergent
-  Amphiphile

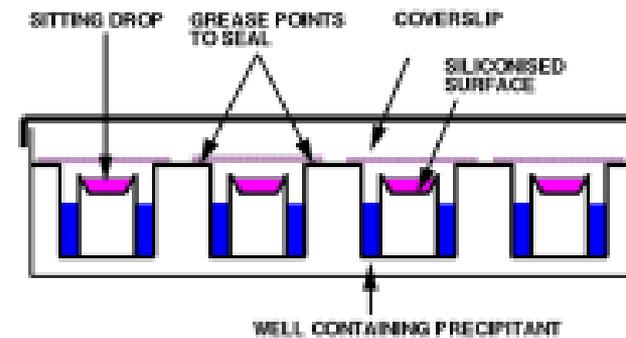


Vapour Diffusion by Hanging or Sitting Drop

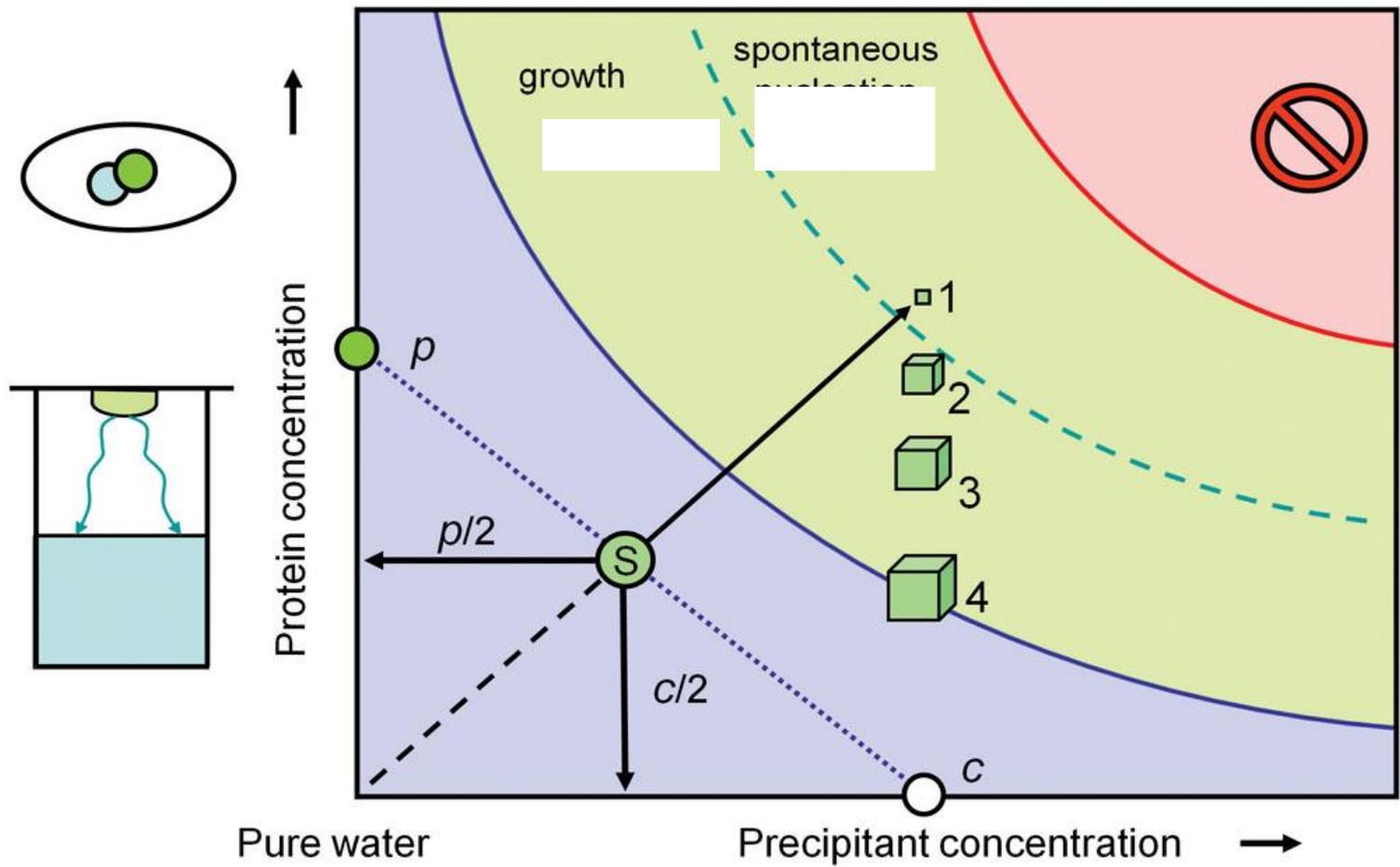
DROP =
1 vol. PROTEIN +
1 vol. PRECIPITANT

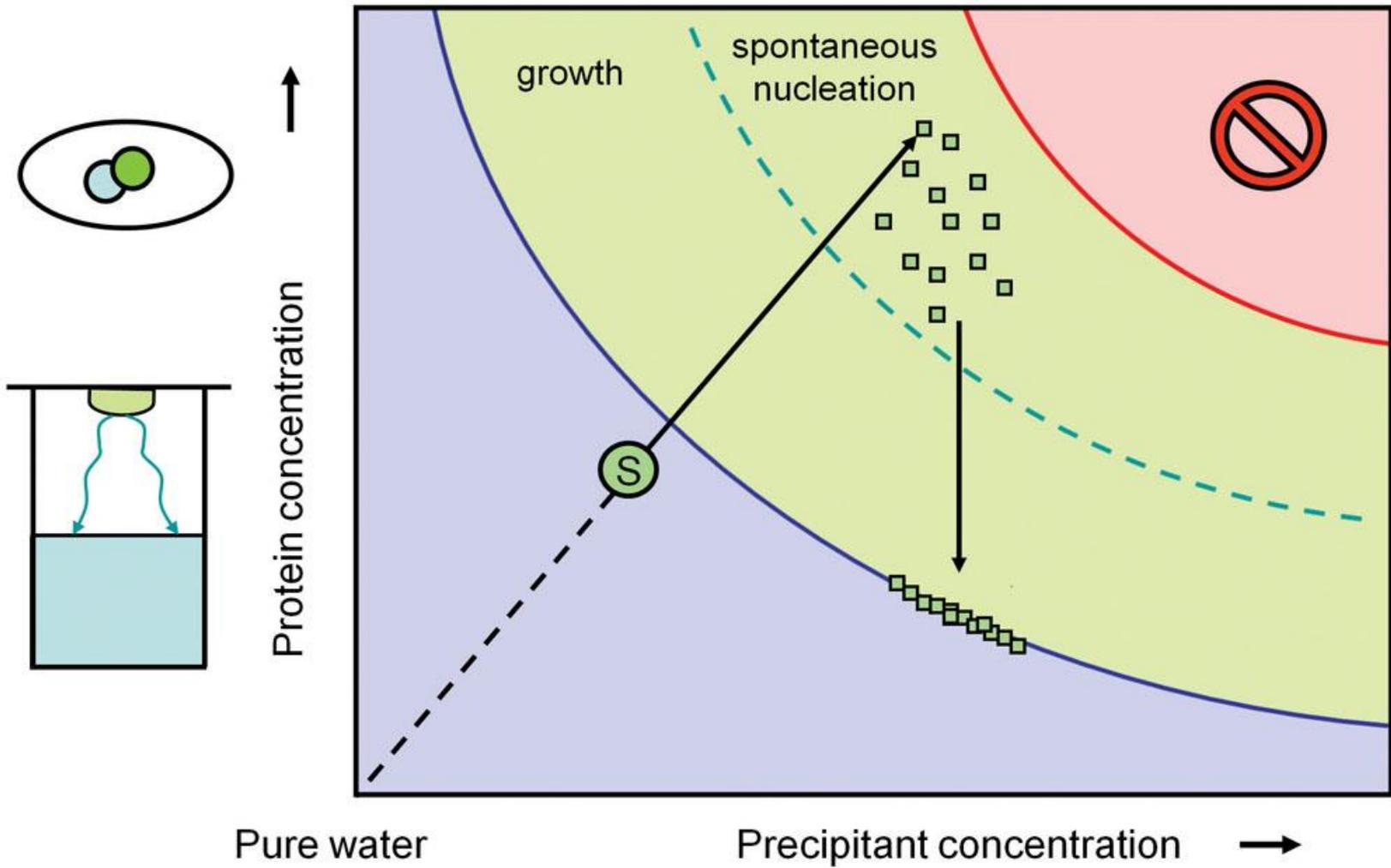


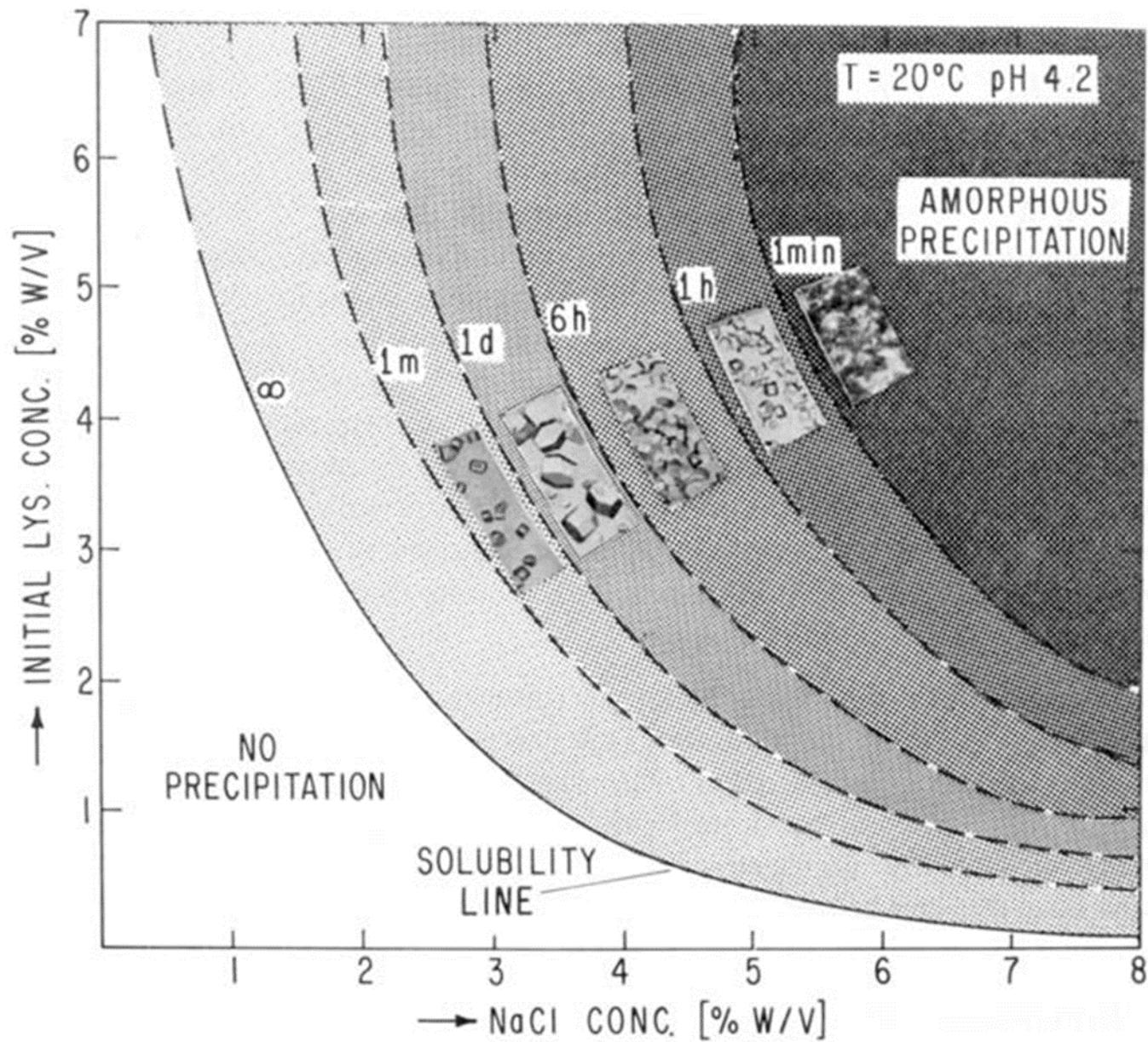
DROP = PROTEIN + PRECIPITANT



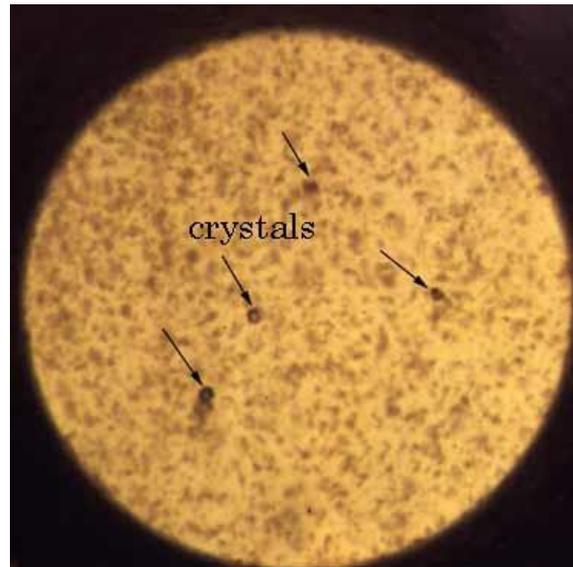
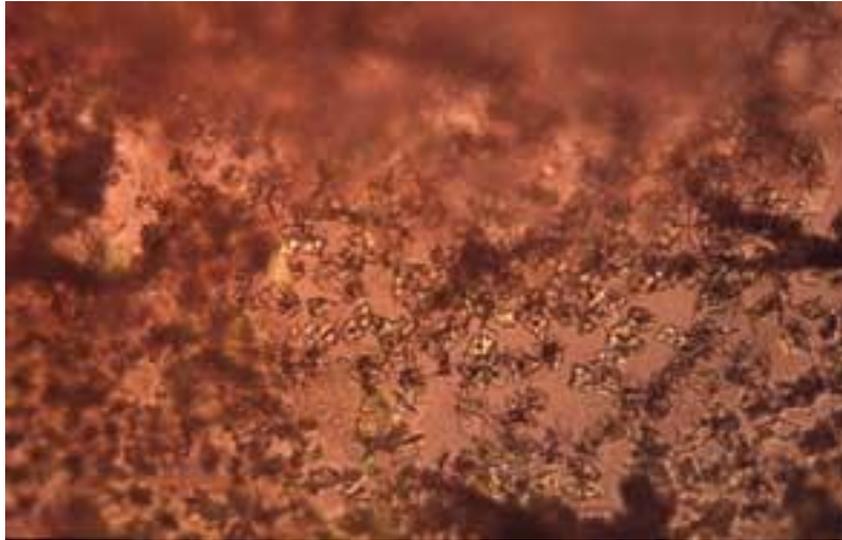
DROP = PROTEIN + PRECIPITANT



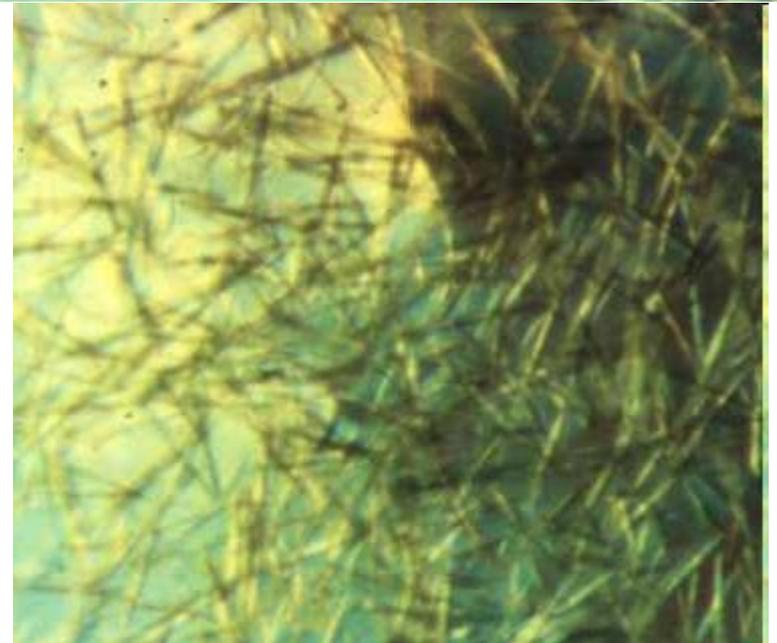
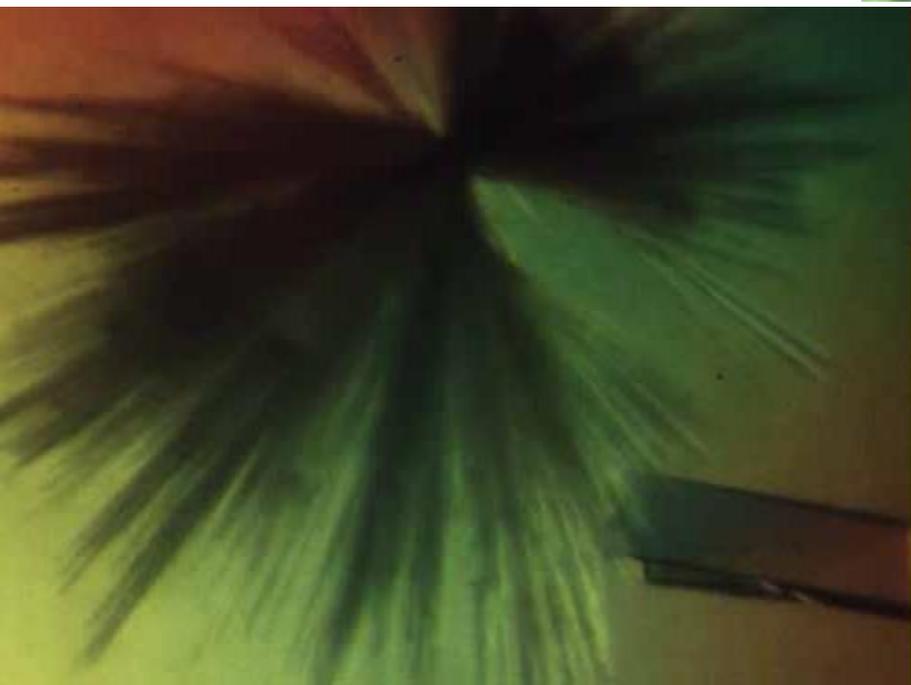
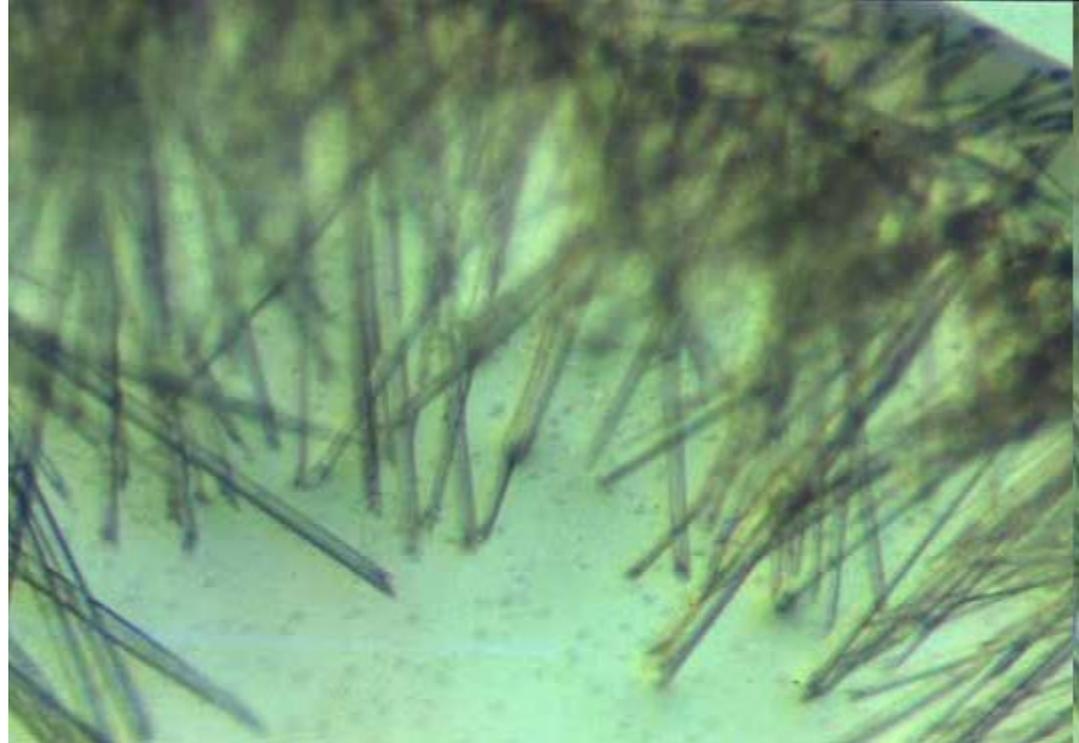




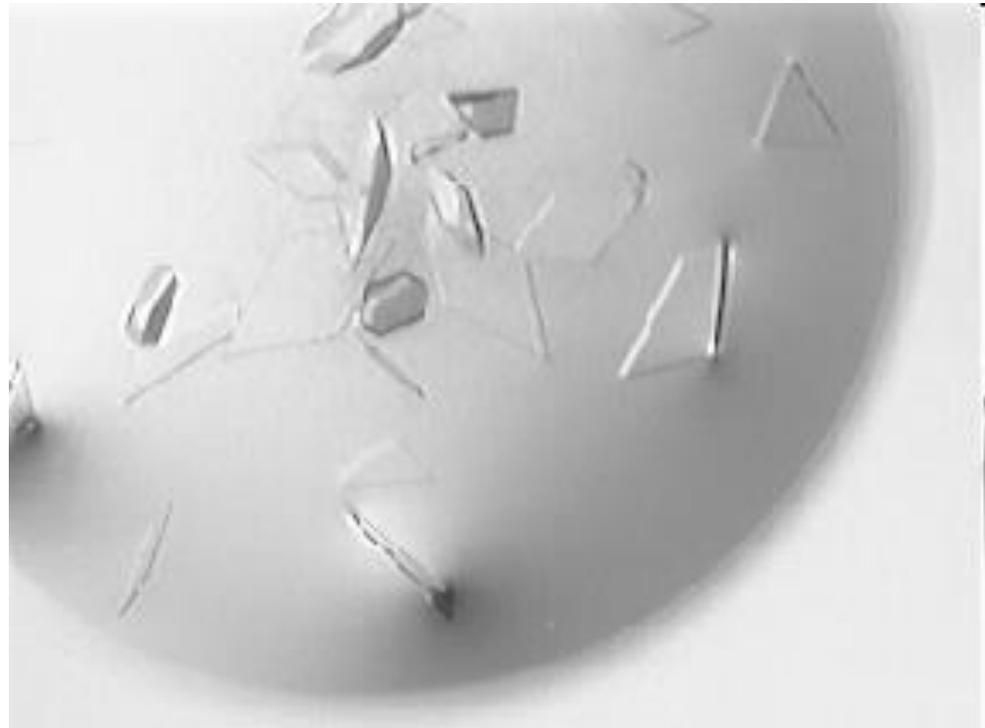
Microcrystalline Precipitate



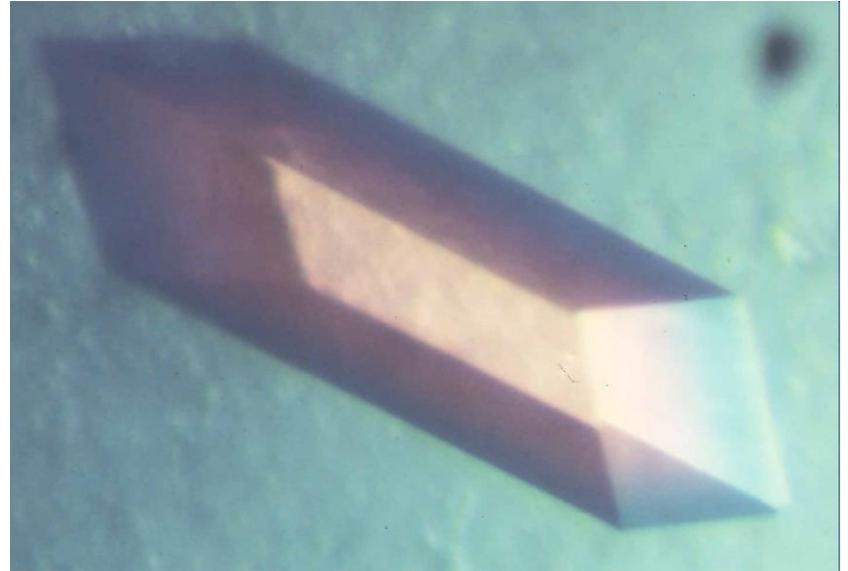
Needles (1-D)

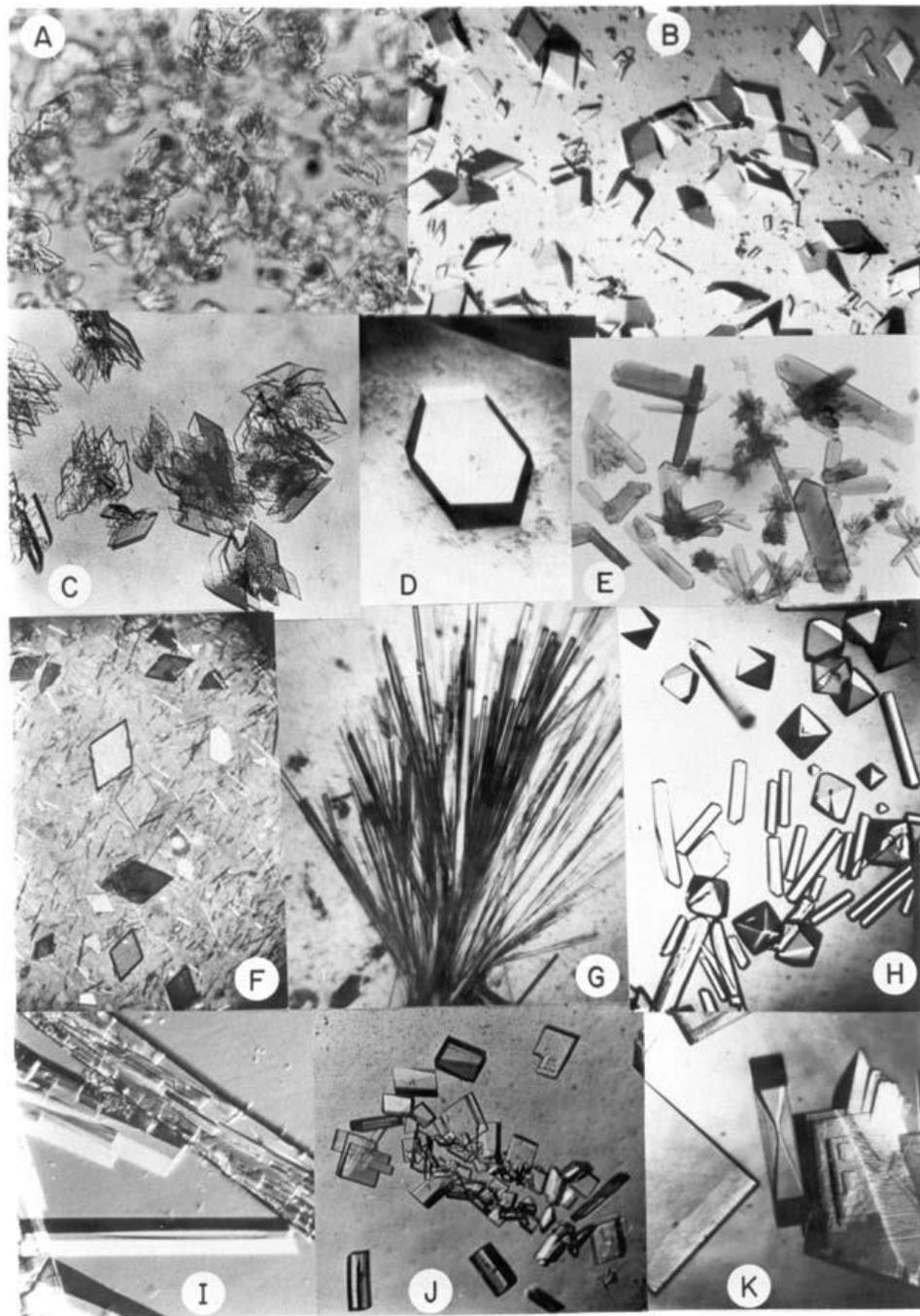


Plates (2-D)

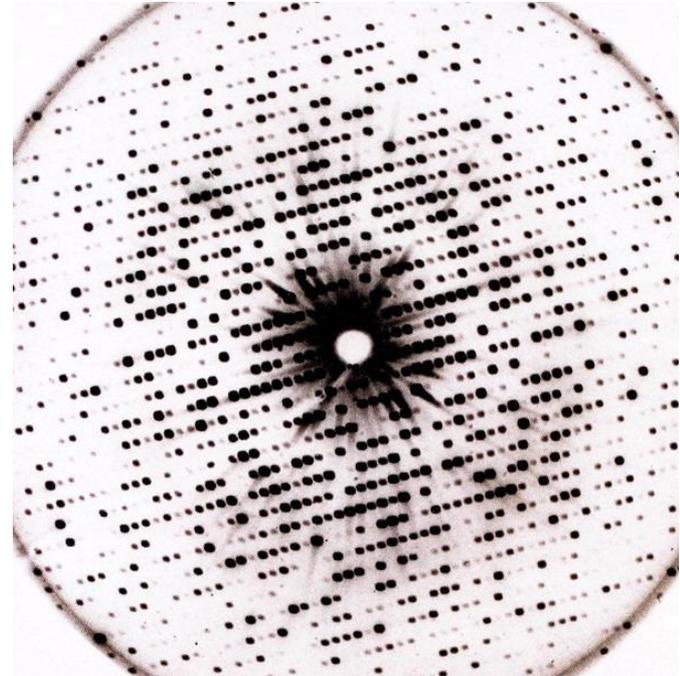
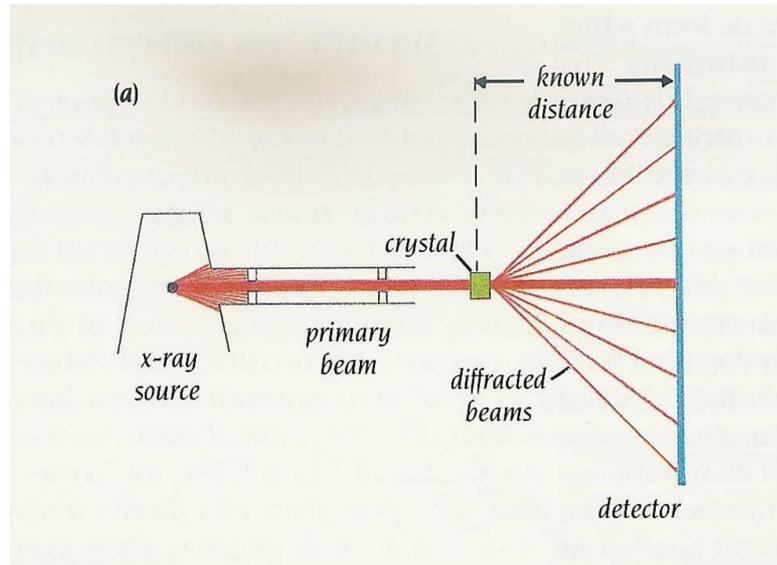


Cristais 3-dimensionaux



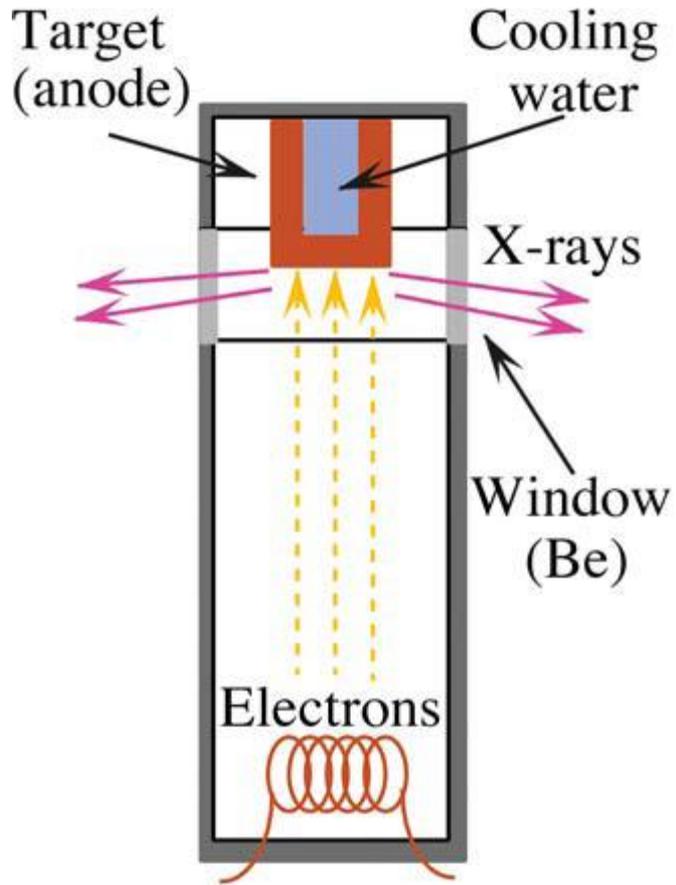


O padrão de difração de raios-X



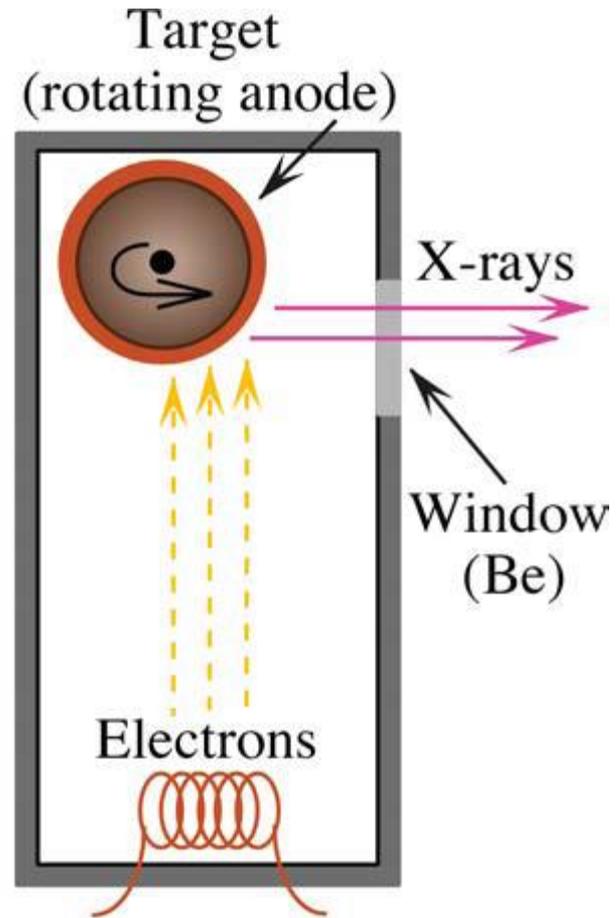
O comprimento de onda dos raios incidentes deve ser da ordem de tamanho de uma ligação química

SEALED TUBE



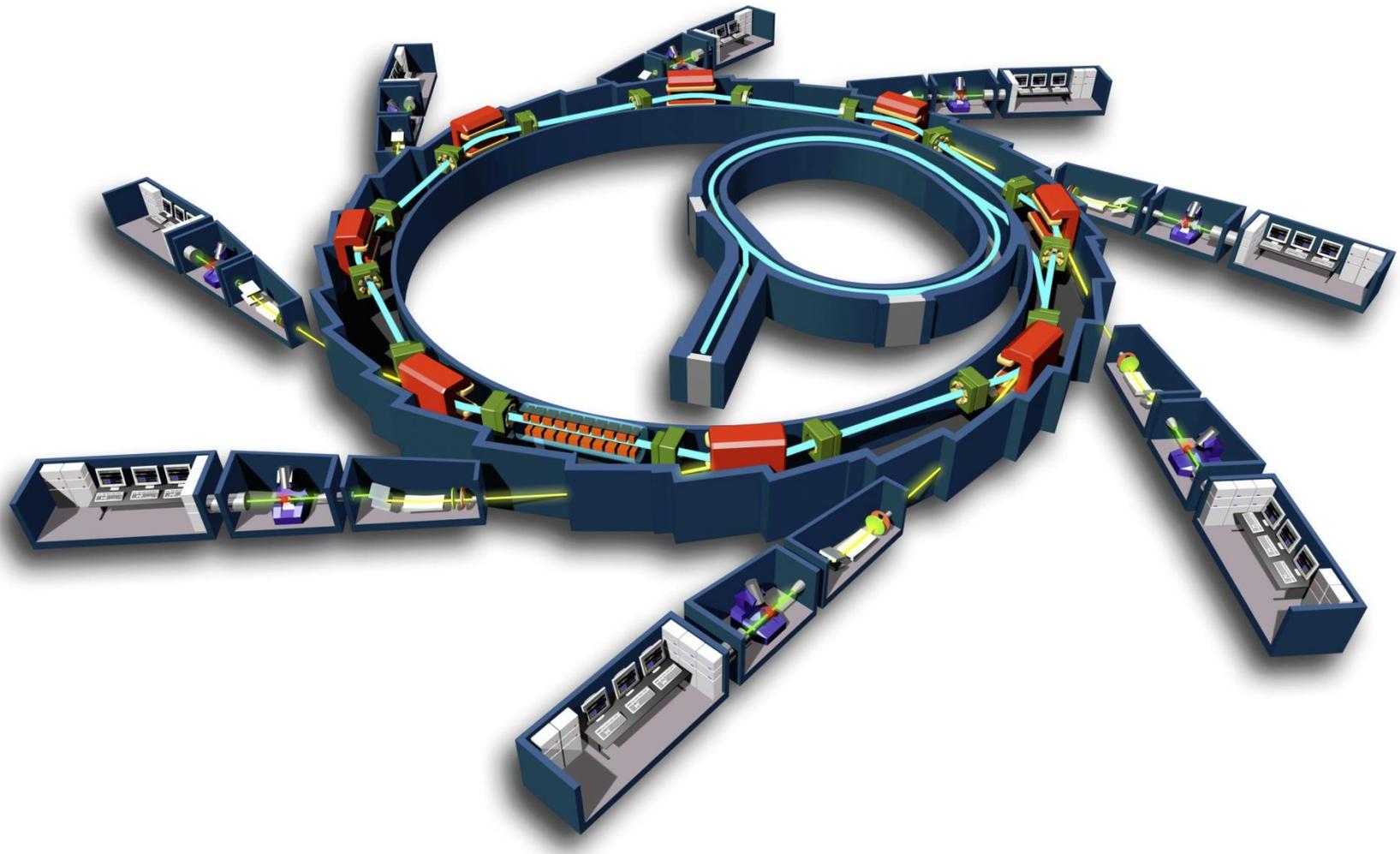
a

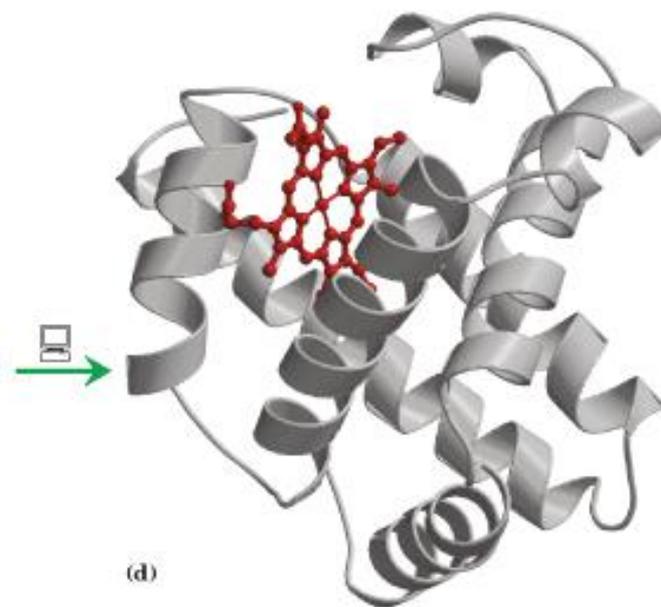
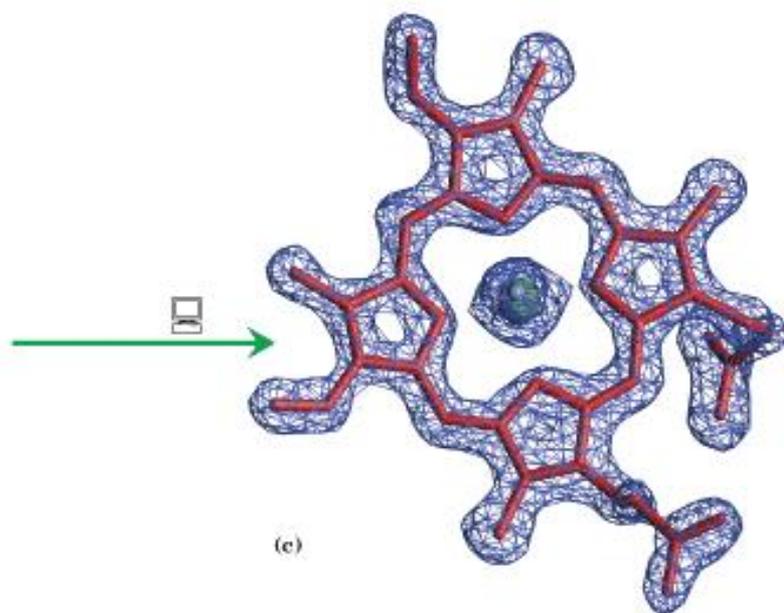
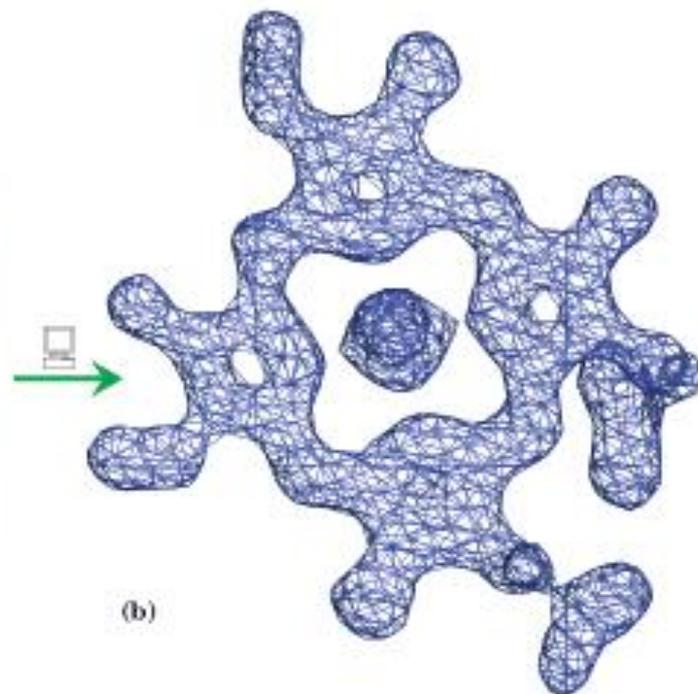
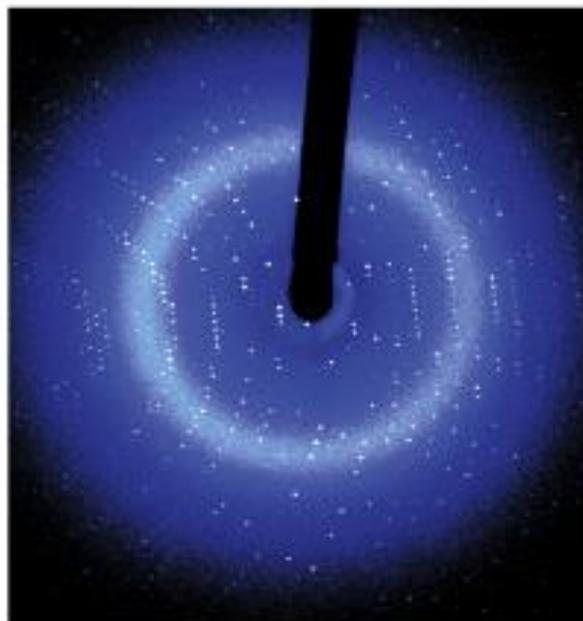
ROTATING ANODE



b

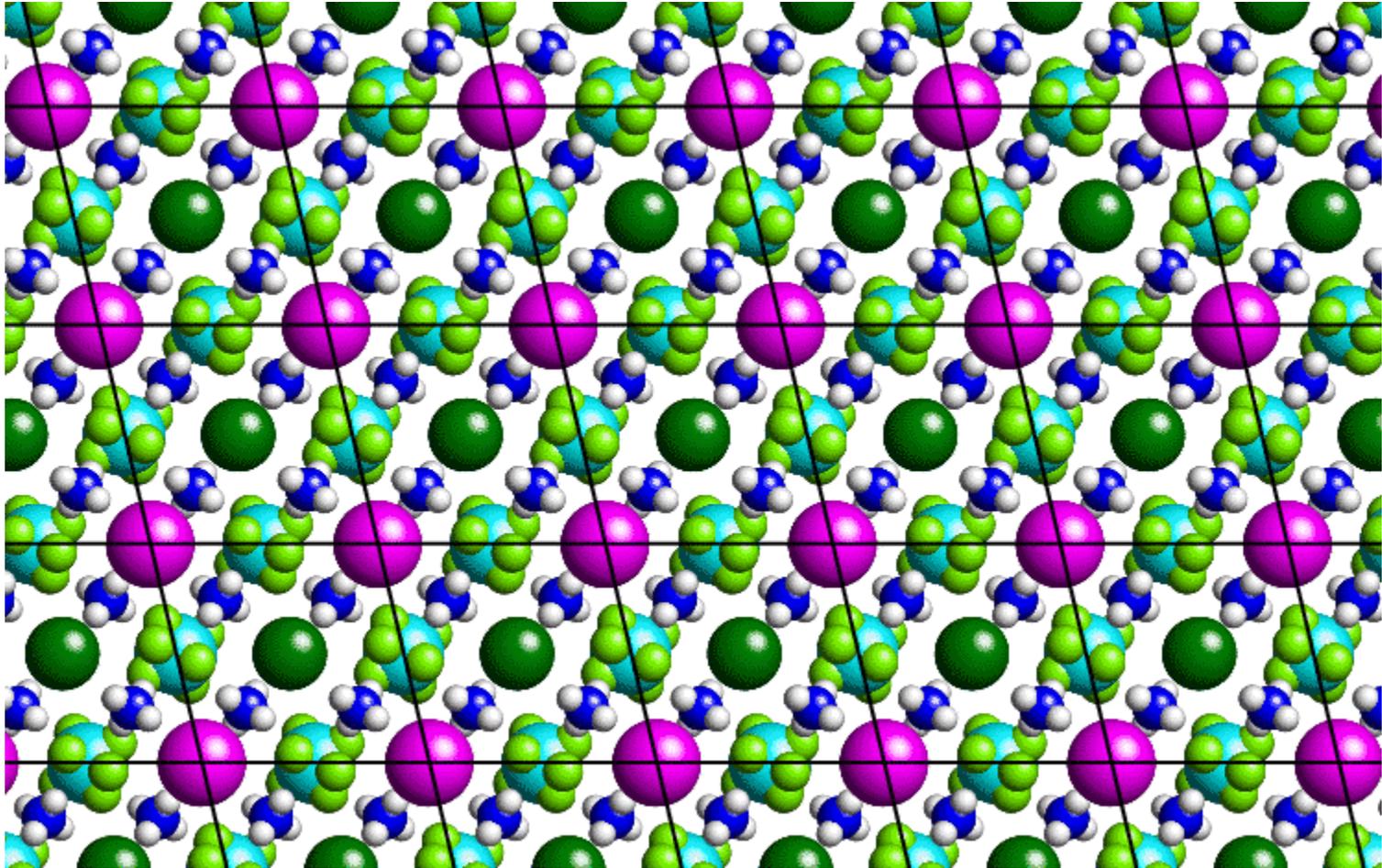
Sincrotrons





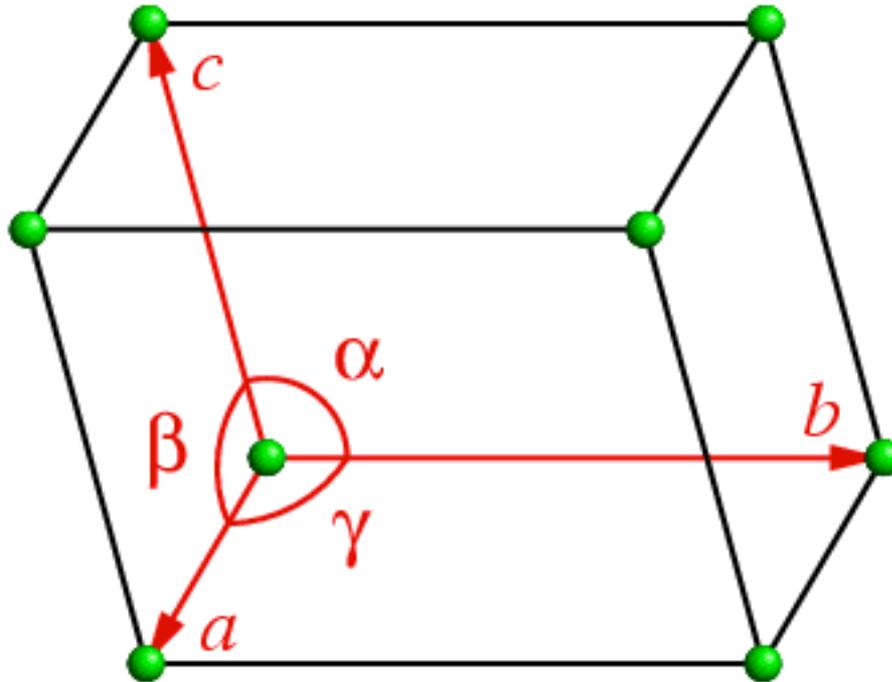
PARTE 2

A rede cristalina e simetria de translação



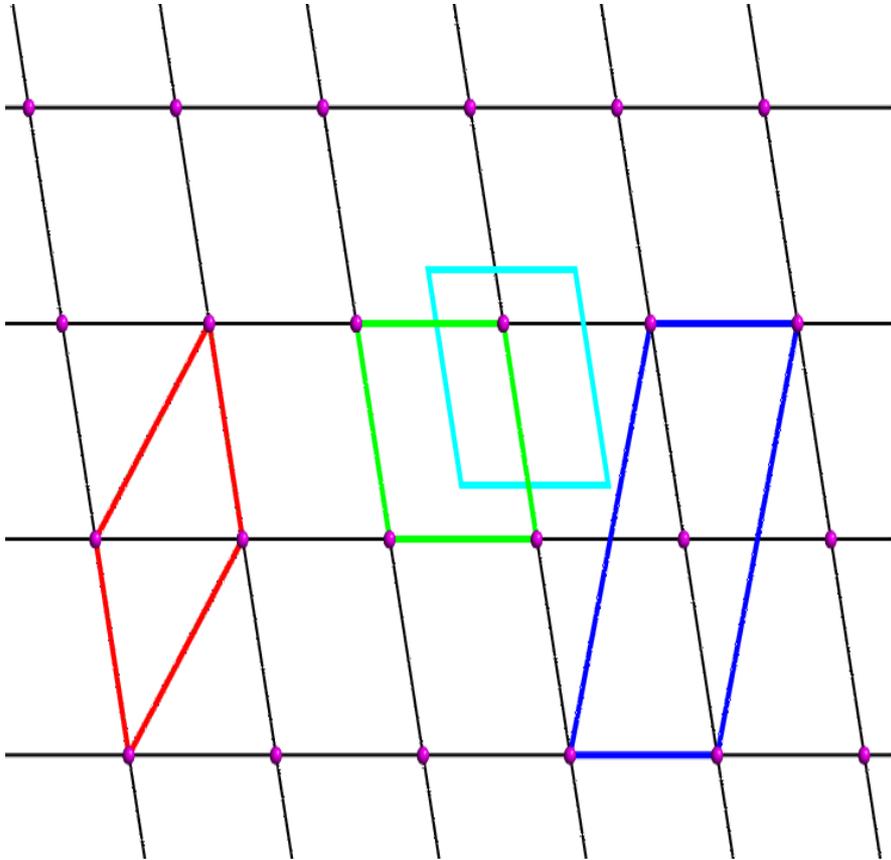
Para descrever a nossa estrutura cristalina, somente precisamos descrever o conteúdo de uma célula unitária mais a simetria de translação da rede (descrita pelos vetores **a**, **b**, **c**)

A célula unitária



Podemos expressar a posição de um ponto (x, y, z) dentro da célula empregando coordenadas em \AA (Ångstroms) ou em coordenadas fracionais dos vetores \mathbf{a} , \mathbf{b} e \mathbf{c} .
Por exemplo, para uma célula com dimensões $40 \text{ \AA} \times 50 \text{ \AA} \times 100 \text{ \AA}$
O ponto $(30 \text{ \AA}, 25 \text{ \AA}, 20 \text{ \AA})$ é o mesmo do ponto $(0.75, 0.5, 0.2)$ em coordenadas fracionais

Escolhendo a célula unitária



<u>Centring Type</u>	<u>Symbol</u>	<u>Multiplicity</u>
<u>Primitive - no centring</u>	<u>P</u>	<u>1</u>
<u>A-face centred</u>	<u>A</u>	<u>2</u>
<u>B-face centred</u>	<u>B</u>	<u>2</u>
<u>C-face centred</u>	<u>C</u>	<u>2</u>
<u>All-face centred</u>	<u>F</u>	<u>4</u>
<u>Body centred</u>	<u>I</u>	<u>2</u>
<u>Rhombohedrally centred</u>	<u>R</u>	<u>3</u>

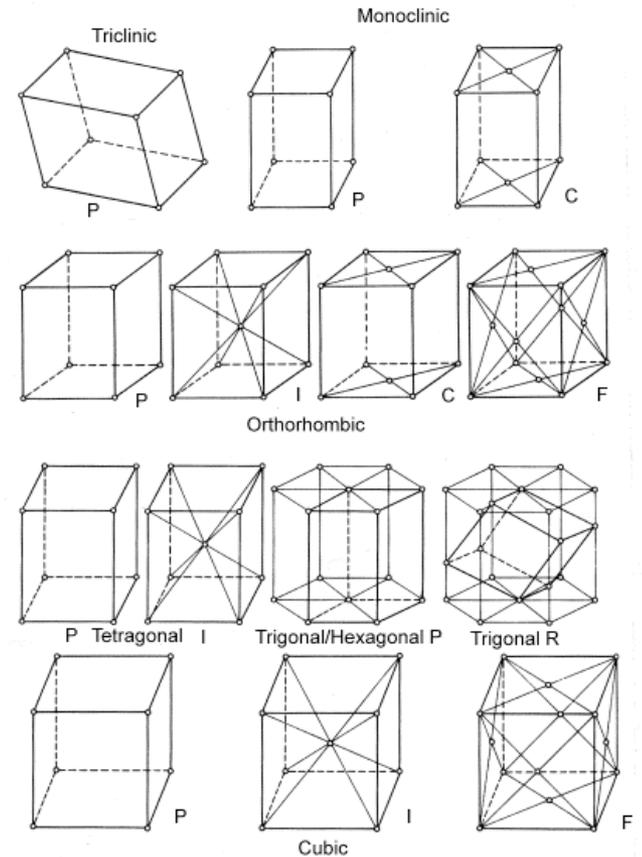
Frequentemente, a origem corresponde a um ponto de alta simetria dentro da célula unitária: por exemplo, num eixo ou na intersecção de dois ou mais eixos.

Normalmente escolhemos células unitárias que contem um pequeno número de pontos de rede e que tem ângulos o mais próximo à 90° possível.

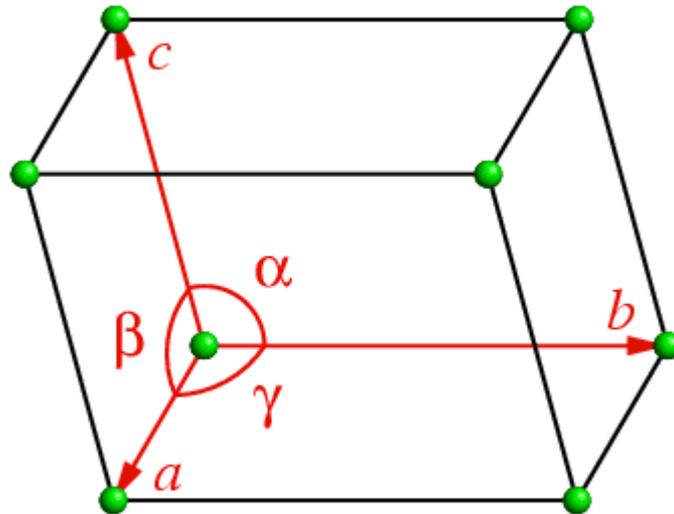
(Multiplicidade: a razão do volume da célula a uma célula primitiva.)

Bravais lattice = crystal system + lattice centering

Crystal family	Lattice system	Centering and 14 Bravais Lattices			
		Primitive	Base-centered	Body-centered	Face-centered
triclinic					
		$\beta \neq 90^\circ$ $a \neq c$	$\beta \neq 90^\circ$ $a \neq c$		
monoclinic					
		$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$
orthorhombic					
		$a \neq c$		$a \neq c$	
tetragonal					
		$\alpha \neq 90^\circ$			
hexagonal	rhombohedral				
	hexagonal	$\gamma = 120^\circ$			
cubic					



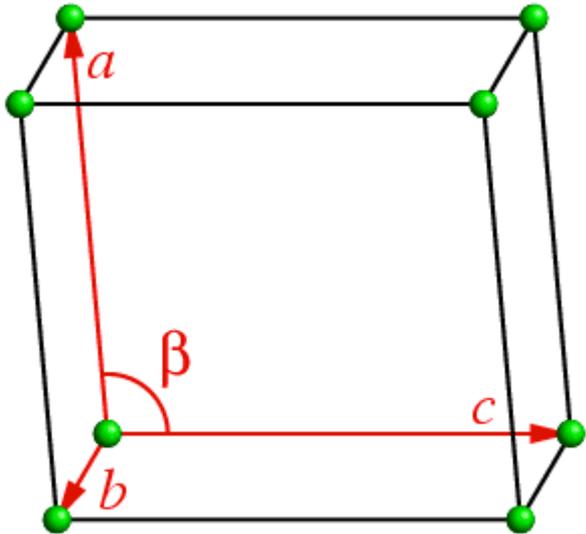
Redes de Bravais Triclinica



aP
triclinico primitivo

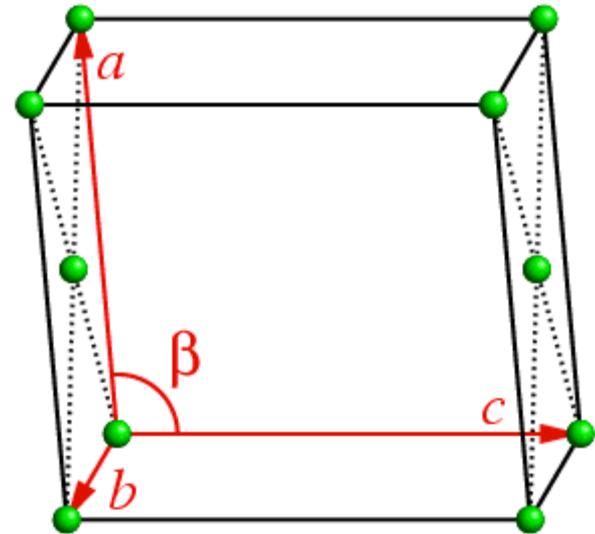
Symbol = crystal system + lattice centring

Redes de Bravais Monoclinicas



mP

Monoclinico primitivo

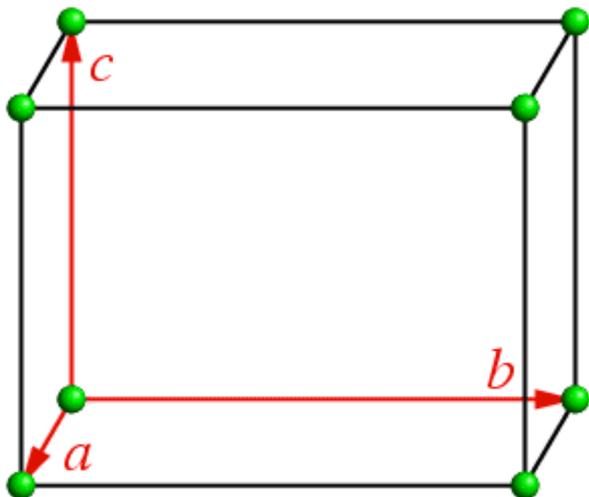


mC

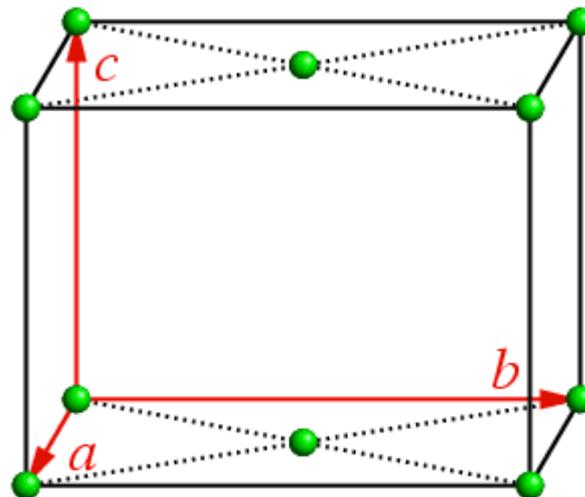
Monoclinico centrado

Symbol = crystal system + lattice centring

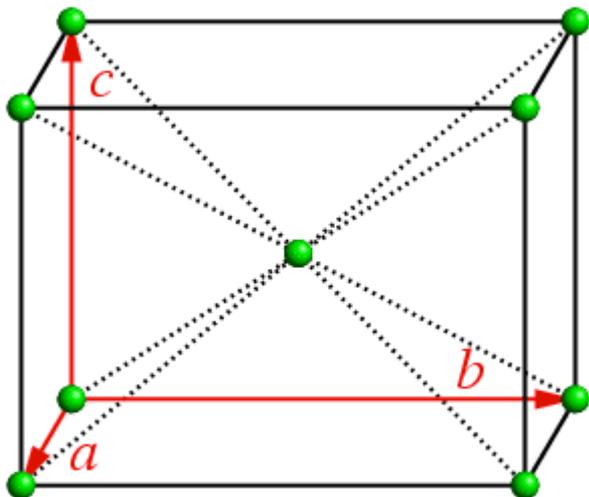
Redes de Bravais Ortorrômbricas



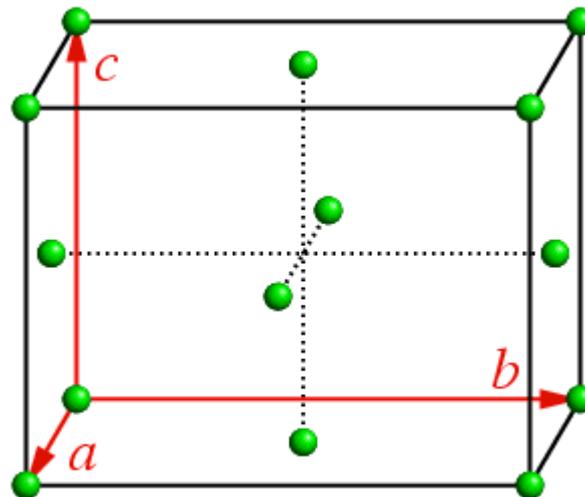
oP



oC

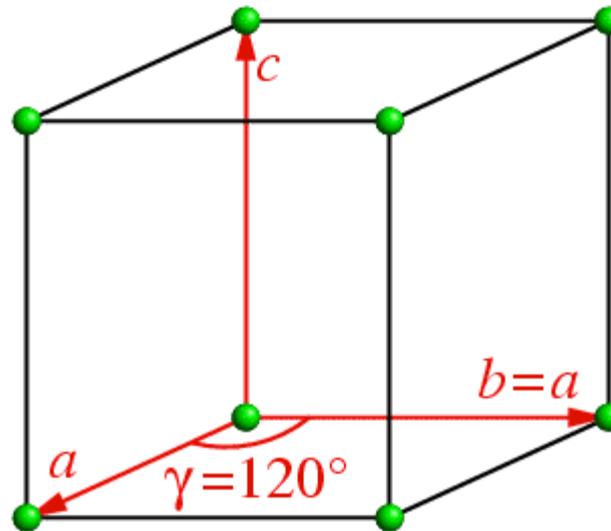


oI



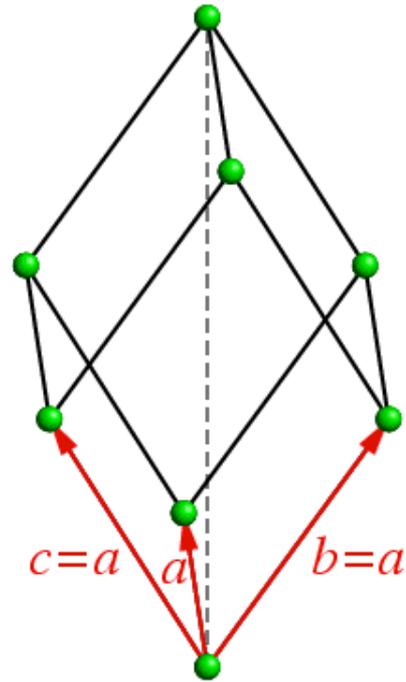
oF

Rede de Bravais Hexagonal



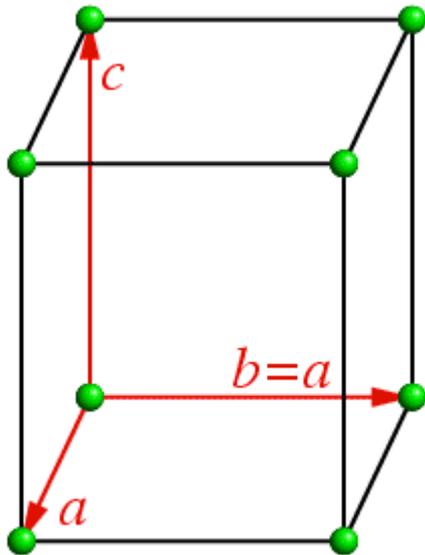
hP

Rede de Bravais Rhombohedral

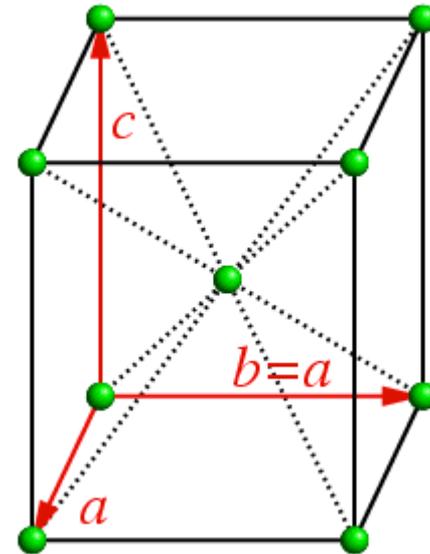


hR

Rede de Bravais Tetragonal



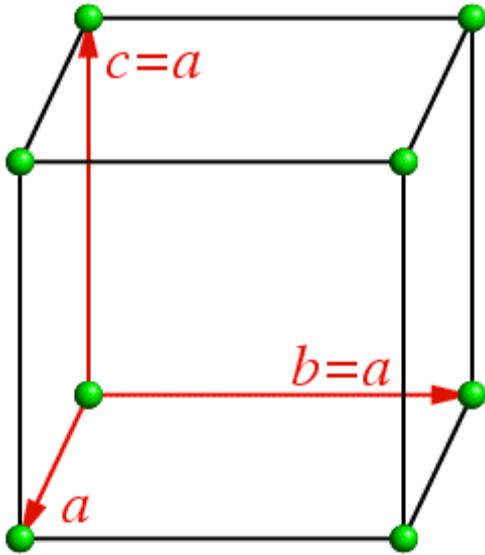
tP



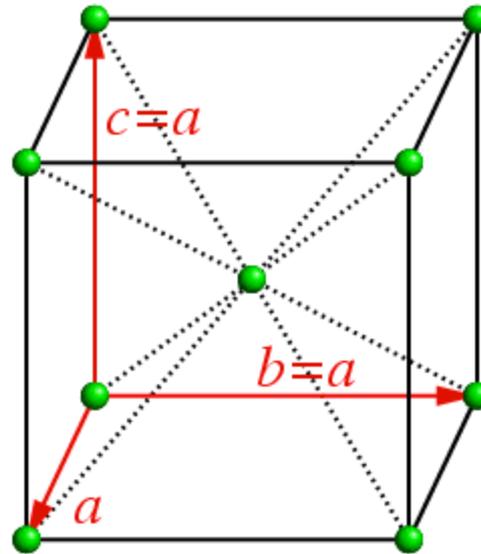
tI

Eixo de ordem 4 na direção c

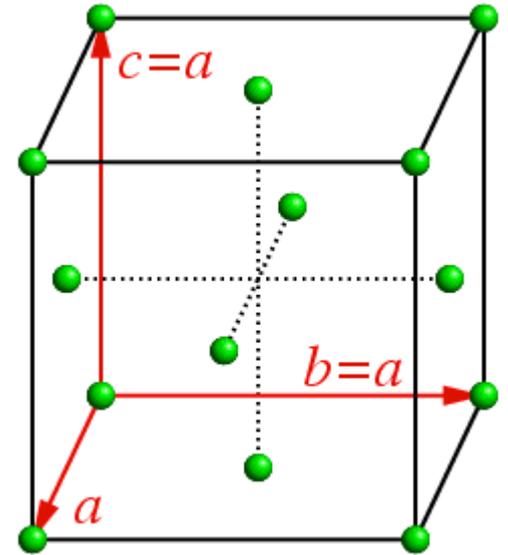
Redes de Bravais Cúbicas



cP



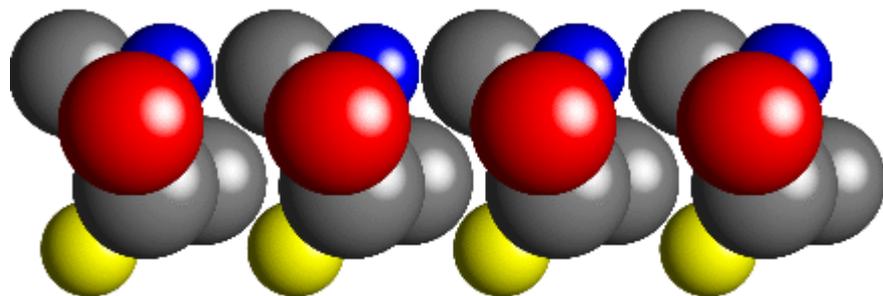
cI



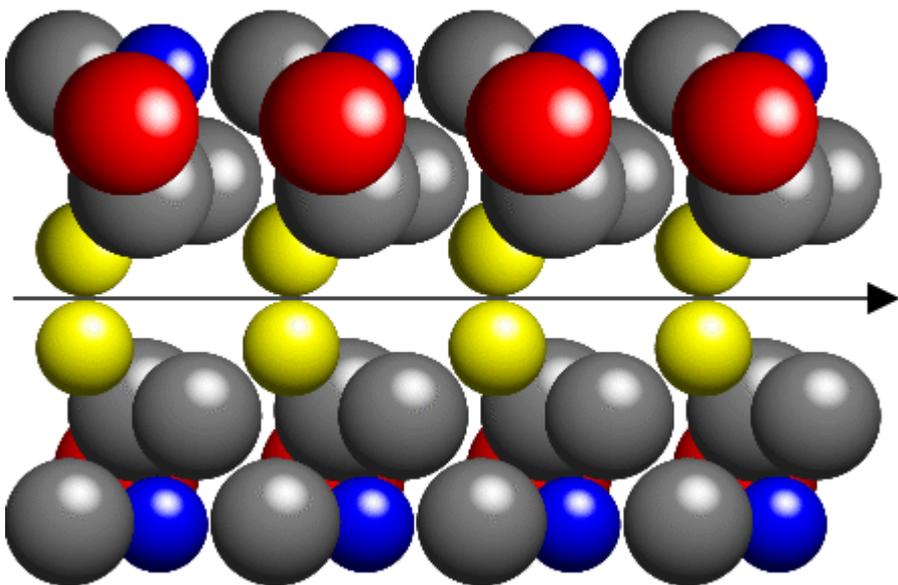
cF

Eixos de ordem 2 paralelos ao a, b e c
e eixos diagonais de ordem 3.

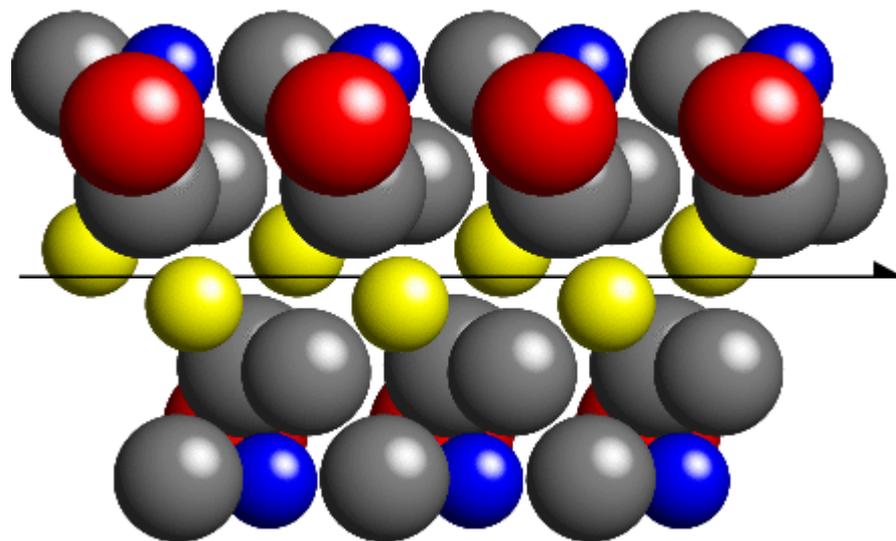
Elementos Internos de Simetria



Simetria translacional

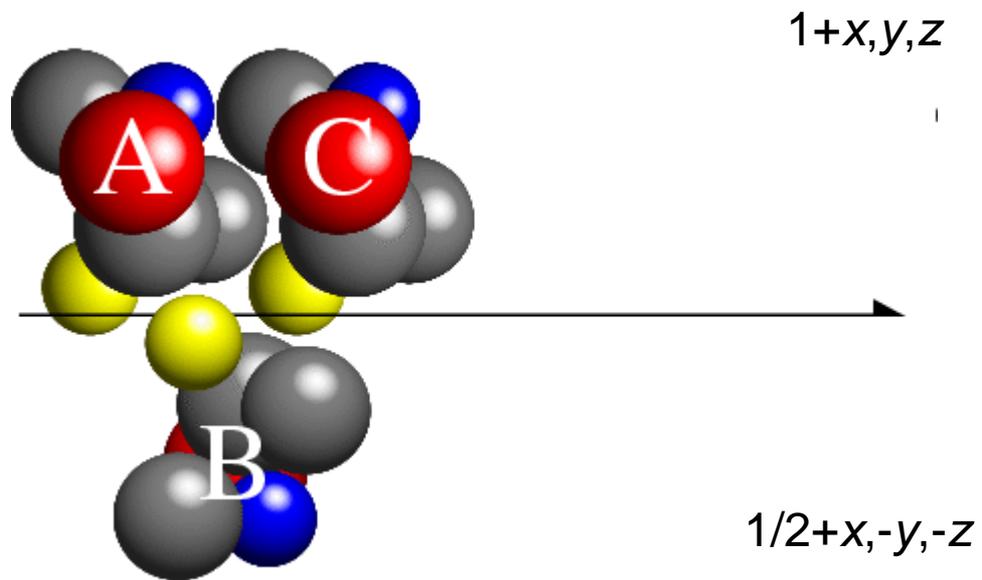


Eixo de ordem 2

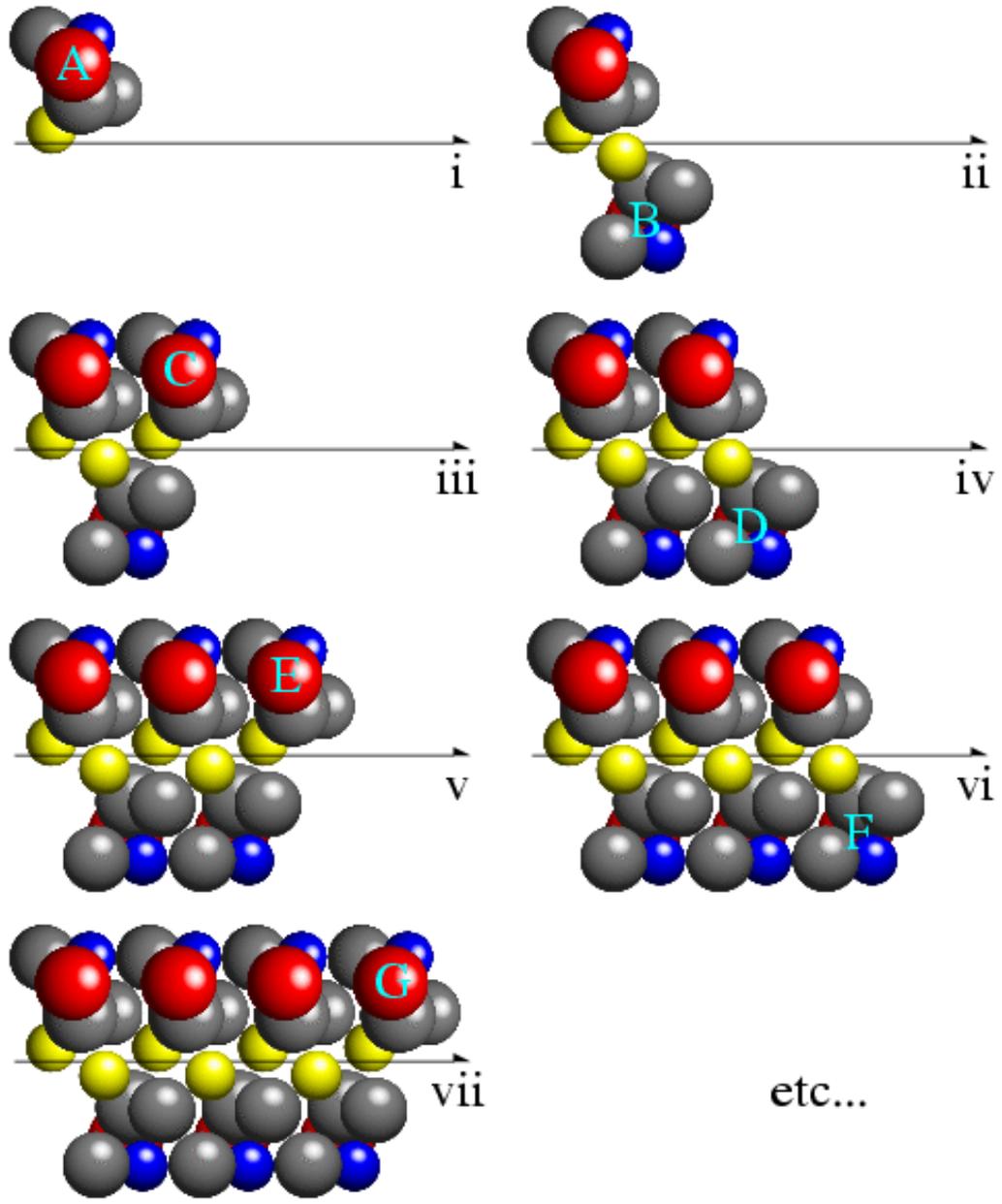


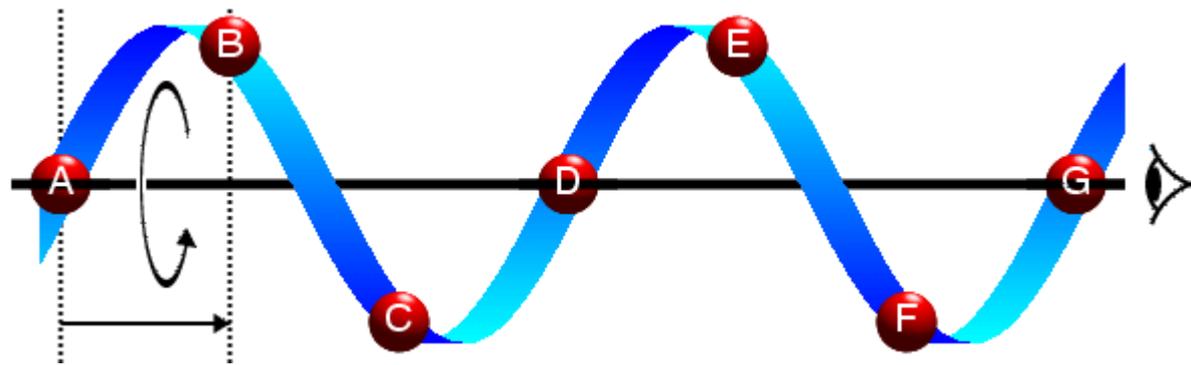
Eixo de parafuso de ordem 2₁

Eixo de ordem 2_1

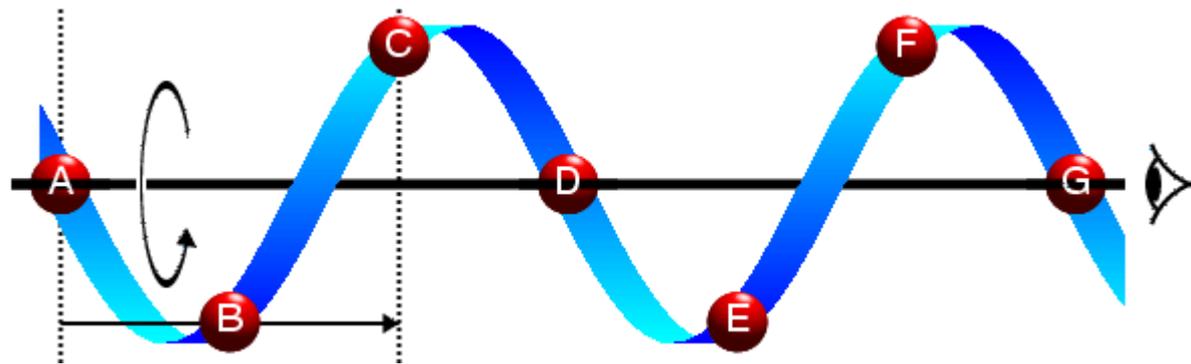


Operador de simetria





3_1



3_2

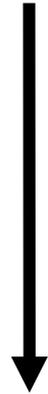
Ordem Eixo de parafuso

2	2_1
3	$3_1, 3_2$
4	$4_1, 4_2, 4_3$
6	$6_1, 6_2, 6_3, 6_4, 6_5$

Grupos Espaciais

A simetria do grupo espacial é uma combinação da simetria translacional da rede em combinação com outros elementos de simetria como rotação e/ou eixos de parafuso.

230 grupos espaciais cristalográficos em 3 dimensões.



**Proteínas são
assimétricas**

**65 grupos espaciais enantiomórficos são permitidos
para macromoléculas quirais**

Crystal System	Laue Class	Crystal Class	Lattice Centring	Enantiomorphic Space Groups	Number of Asymmetric Units per Unit Cell
Triclinic	-1	1	<i>P</i>	<i>P</i> 1	1
Monoclinic	<i>2/m</i>	2	<i>P</i>	<i>P</i> 2, <i>P</i> 2 ₁	2
			<i>C</i>	<i>C</i> 2	4
Orthorhombic	<i>mmm</i>	222	<i>P</i>	<i>P</i> 222, <i>P</i> 222 ₁ , <i>P</i> 2 ₁ 2 ₁ 2, <i>P</i> 2 ₁ 2 ₁ 2 ₁	4
			<i>C</i>	<i>C</i> 222, <i>C</i> 222 ₁	8
			<i>F</i>	<i>F</i> 222	16
			<i>I</i>	<i>I</i> 222, <i>I</i> 2 ₁ 2 ₁ 2 ₁	8
Tetragonal	<i>4/m</i>	4	<i>P</i>	<i>P</i> 4, <i>P</i> 4 ₁ , <i>P</i> 4 ₂ , <i>P</i> 4 ₃	4
			<i>I</i>	<i>I</i> 4, <i>I</i> 4 ₁	8
	<i>4/mmm</i>	422	<i>P</i>	<i>P</i> 422, <i>P</i> 42 ₁ 2, <i>P</i> 4 ₁ 22, <i>P</i> 4 ₁ 2 ₁ 2, <i>P</i> 4 ₂ 22, <i>P</i> 4 ₂ 2 ₁ 2, <i>P</i> 4 ₃ 22, <i>P</i> 4 ₃ 2 ₁ 2	8
			<i>I</i>	<i>I</i> 422, <i>I</i> 42 ₁ 2	16
Trigonal (see note)	-3	3	<i>P</i>	<i>P</i> 3, <i>P</i> 3 ₁ , <i>P</i> 3 ₂	3
			<i>R</i>	<i>R</i> 3	9
	-3 <i>m</i>	312	<i>P</i>	<i>P</i> 312, <i>P</i> 3 ₁ 12, <i>P</i> 3 ₂ 12	6
		321	<i>R</i>	<i>P</i> 321, <i>P</i> 3 ₁ 21, <i>P</i> 3 ₂ 21	6
Hexagonal	<i>6/m</i>	6	<i>P</i>	<i>P</i> 6, <i>P</i> 6 ₁ , <i>P</i> 6 ₂ , <i>P</i> 6 ₃ , <i>P</i> 6 ₄ , <i>P</i> 6 ₅	6
	<i>6/mmm</i>	622	<i>P</i>	<i>P</i> 622, <i>P</i> 6 ₁ 22, <i>P</i> 6 ₂ 22, <i>P</i> 6 ₃ 22, <i>P</i> 6 ₄ 22, <i>P</i> 6 ₅ 22	12
Cubic	<i>m-3</i>	23	<i>P</i>	<i>P</i> 23, <i>P</i> 2 ₁ 3	12
			<i>F</i>	<i>F</i> 23	48
			<i>I</i>	<i>I</i> 23, <i>I</i> 2 ₁ 3	24
			<i>P</i>	<i>P</i> 432, <i>P</i> 4 ₂ 32, <i>P</i> 4 ₃ 32, <i>P</i> 4 ₁ 32	24
			<i>F</i>	<i>F</i> 432, <i>F</i> 4 ₁ 32	96
	<i>I</i>	<i>I</i> 432, <i>I</i> 4 ₁ 32	48		

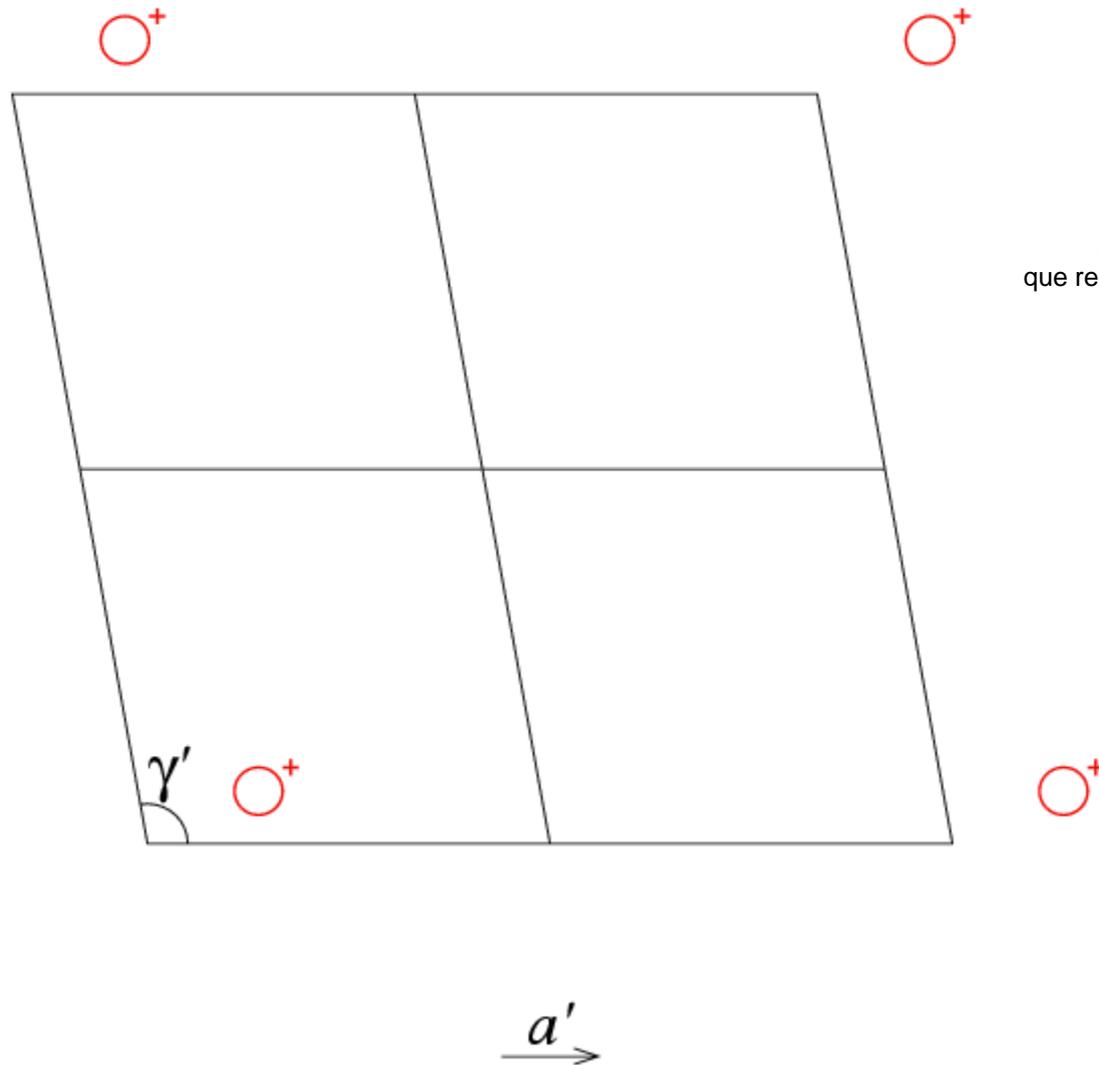
Diagramas de grupos espaciais - TRICLINIC (P1)

*P*1

P 1

1

No. 1

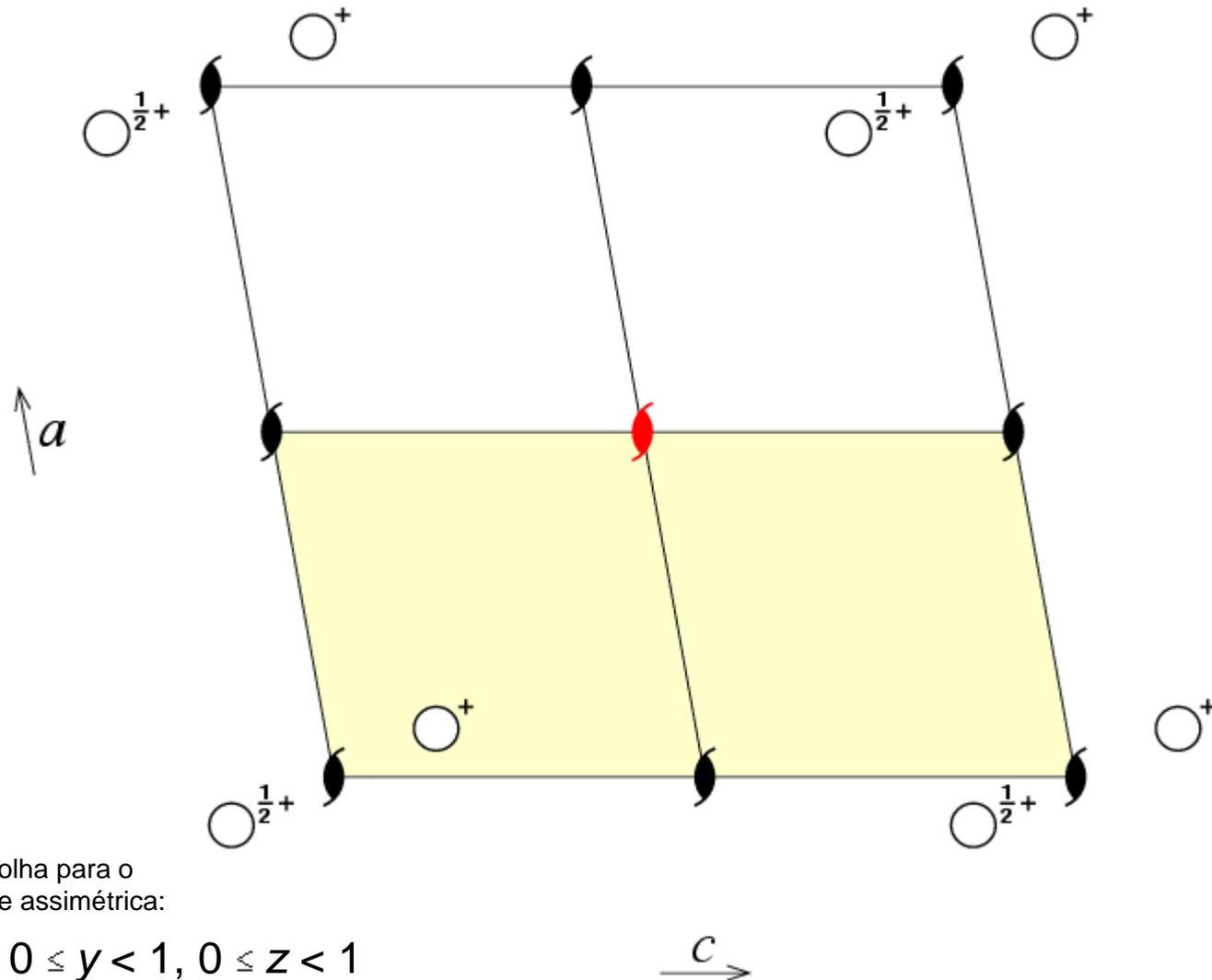


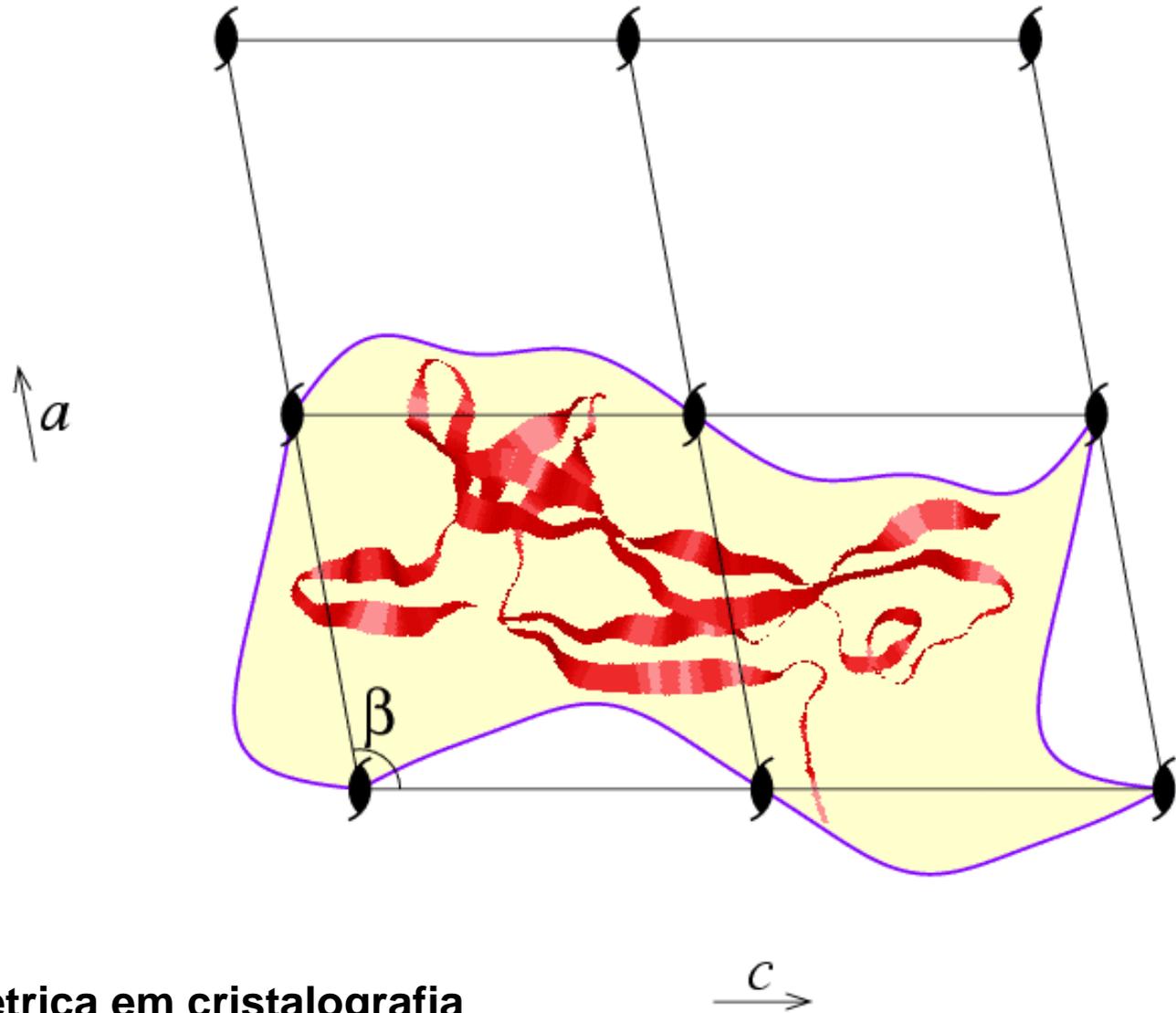
(Operações de simetria
que relacionam pontos equivalentes)

↓
1 x, y, z

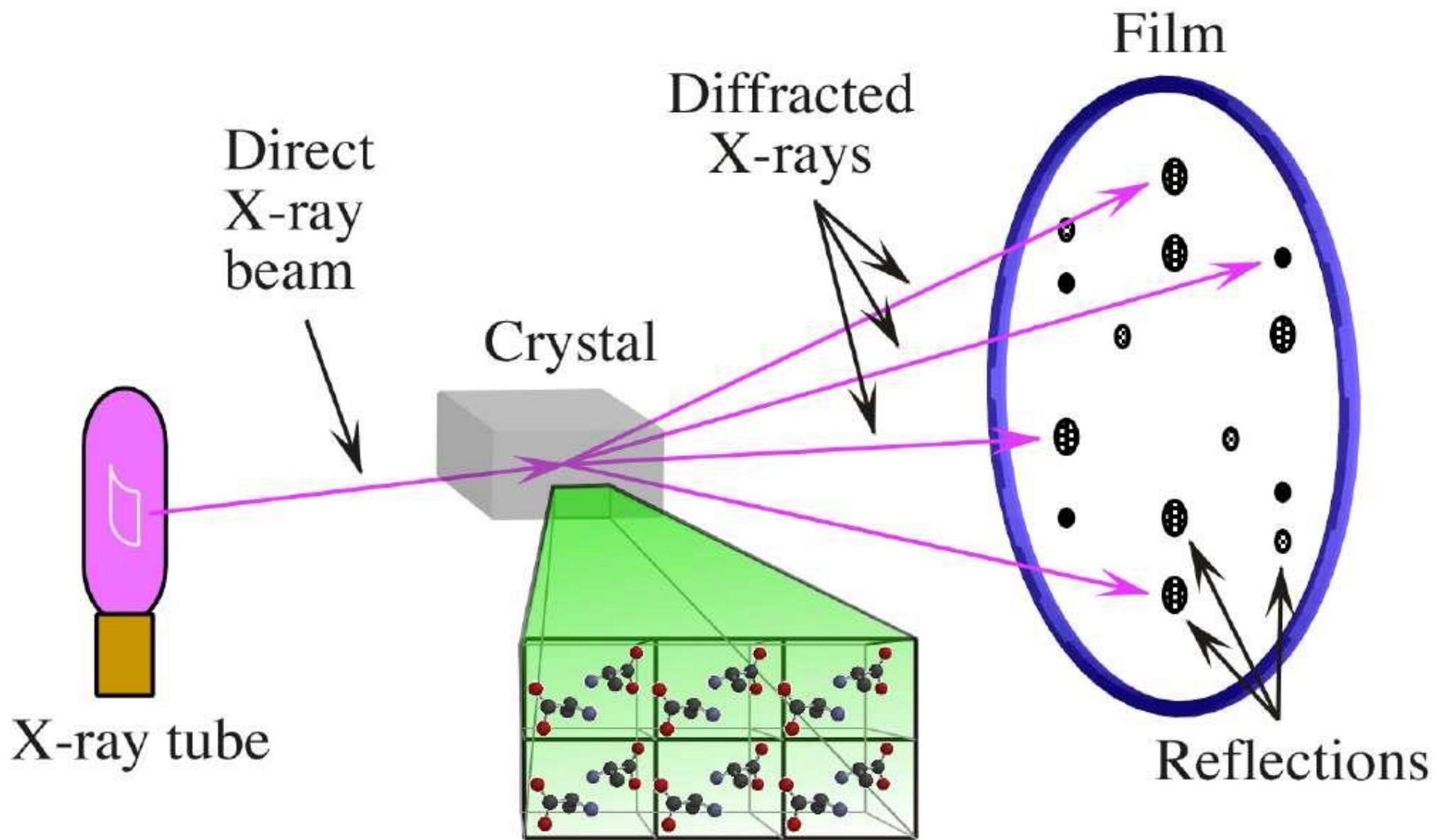
Unidade Assimétrica

A unidade assimétrica de um grupo espacial é a parte da célula unitária que pode ser usada para gerar a célula inteira através de operações de simetria interna do grupo espacial.



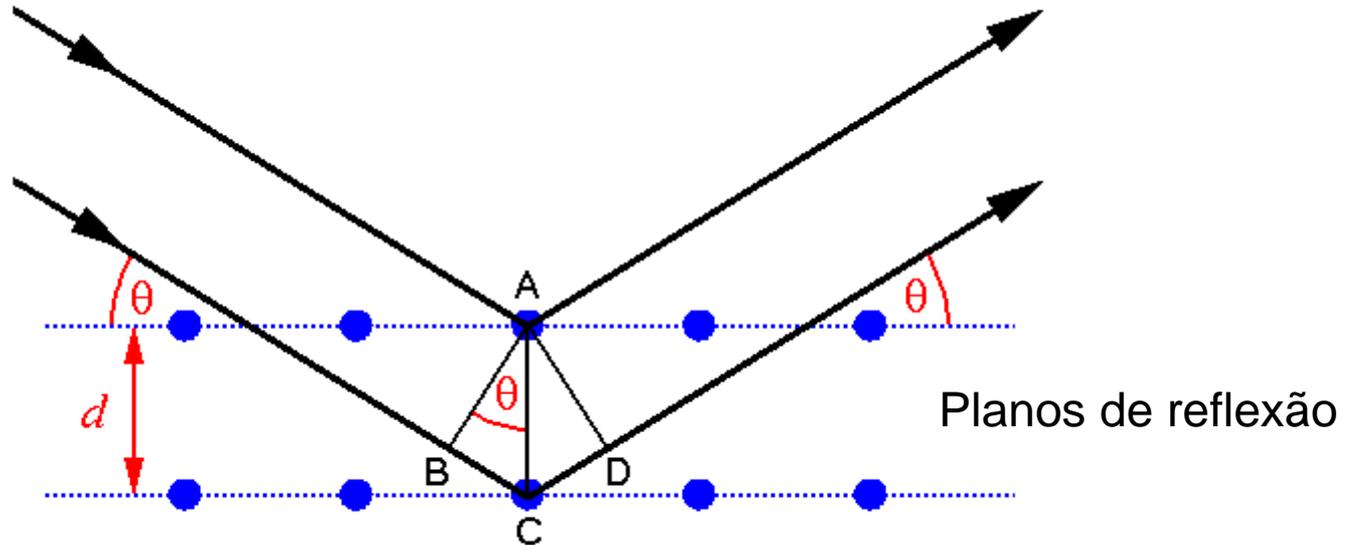


A unidade assimétrica em cristalografia de proteínas é normalmente determinada pela forma da proteína.



Condição para interferência construtiva

$$n\lambda = 2d\sin\theta$$



A diferença de caminho ($2d\sin\theta$) entre ondas que interferem construtivamente é sempre um múltiplo inteiro (n) do comprimento de onda (λ)

Em outras palavras:

A diferença da fase entre ondas que interferem construtivamente é sempre uma múltipla de 2π rad (360°)