X-Ray Crystallography

"If a picture is worth a thousand words, then a macromolecular structure is priceless to a physical biochemist." – van Holde

Topics:

1. Protein Data Bank (PDB)

2. Image Formation

Resolution / Wavelength (Amplitude, Phase) / Light Microscopy / EM / X-ray / (NMR)

2. X-Ray Crystallography

a) Crystal Growth – Materials / Methods

b) Crystal Lattices - Lattice Constants / Space Groups / Asymmetric Unit

c) X-ray Sources – Sealed Tube / Rotation Anode / Synchrotron

d)Theory of Diffraction – Bragg's Law / Reciprocal Space

e) Data Collection – Methods / Detectors / Structure Factors

f) Structure Solution – Phase Problem: MIR / MR / MAD

h) Refinements and Models

i) Analysis and presentation of results

PDB Holdings List: 5-Apr-2005

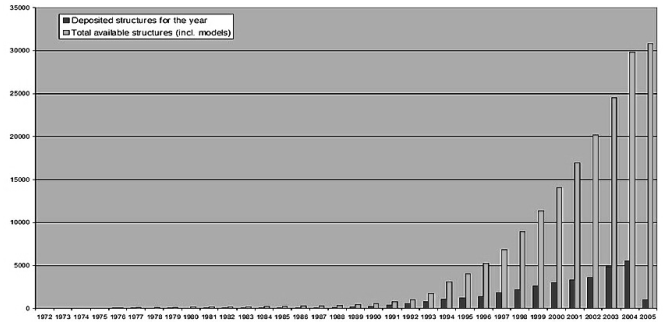
		Molecule Type				
		Proteins, Peptides, and Viruses	Protein/Nucleic Acid Complexes	Nucleic Acids	Carbohydrates	Total
Exp.	X-ray Diffraction and other	23942	1147	778	11	25878
	NMR	3721	111	649	2	4483
Tech.	Total	27663	1258	1427	13	30361

Please note that theoretical models have been removed, effective July 02, 2002, as per PDB policy.

16255 Structure Factor Files

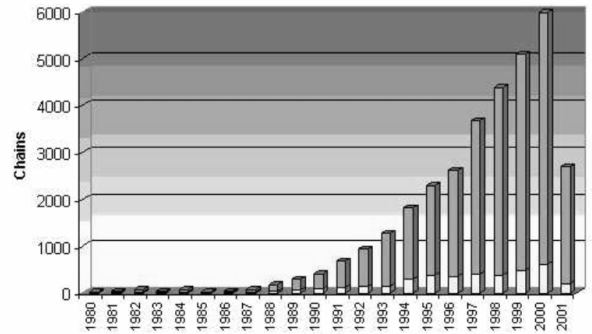
2484 NMR Restraint Files

PDB Content Growth



Protein Data Bank - 17,679 Structures - March 2002

X-ray - 14595
NMR - 2706 "Old" Folds
Theory - 378 "New" Folds



http://www.rcsb.org/pdb/

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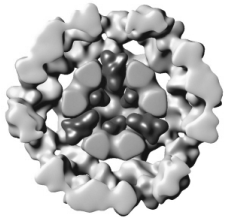
Image Formation

Abbe (~1873): Limit Res. ~ λ/2

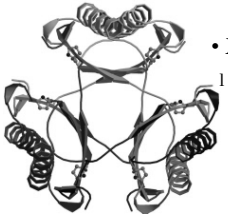
• Light Photography

λ ~ **400 - 700 nm**



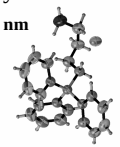
• Electron Microscopy

λ ~ **0.001 - 0.1 nm**



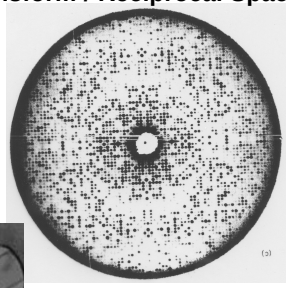
• X-Ray or NMR

λ ~ **0.1 nm**

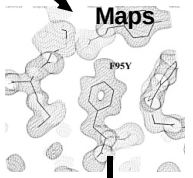


Object → **Transform** → **Image**

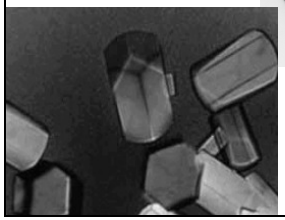
Transform / Reciprocal Space

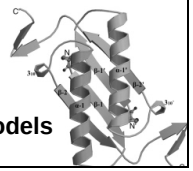


Electron Density Maps



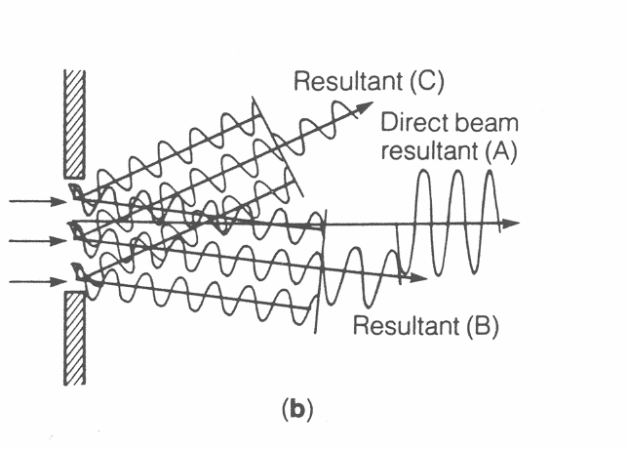
Object / Real Space





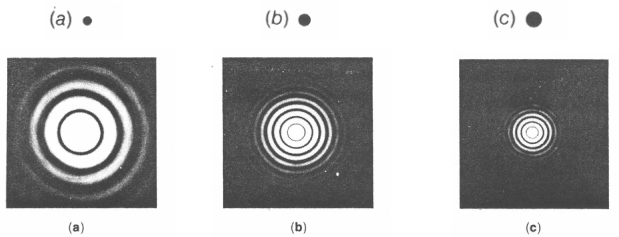
Models

Transforms / Reciprocal Space

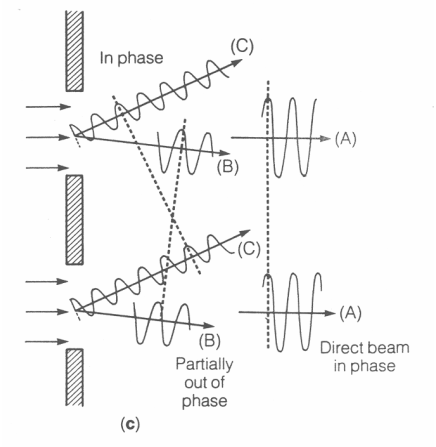


Transforms / Reciprocal Space

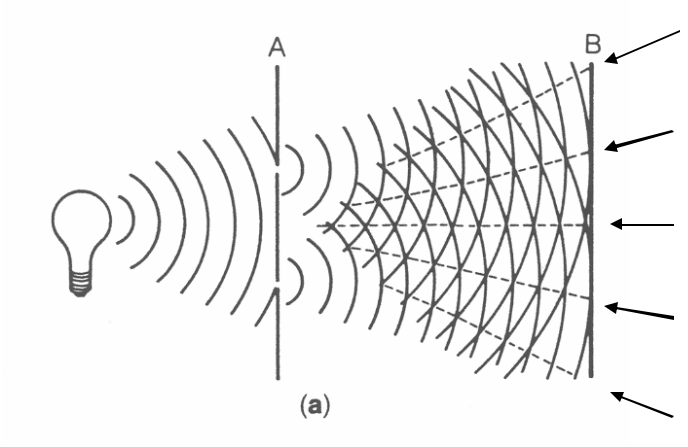
Different size holes



Transforms / Reciprocal Space

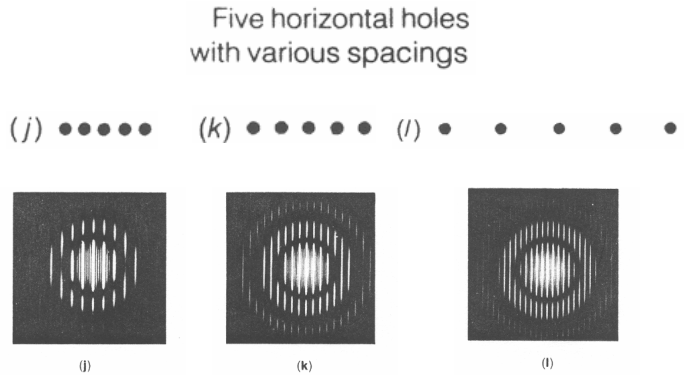


Transforms / Reciprocal Space



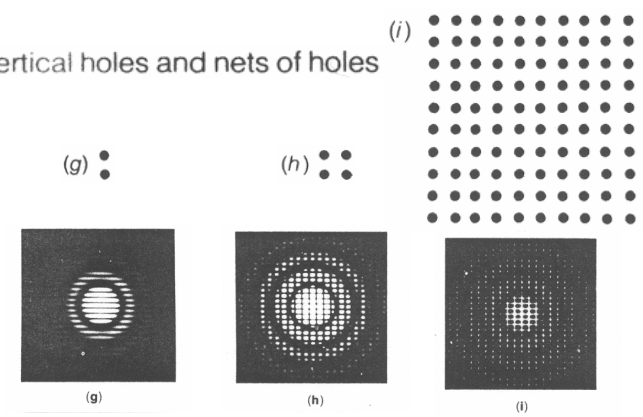
Transforms / Reciprocal Space

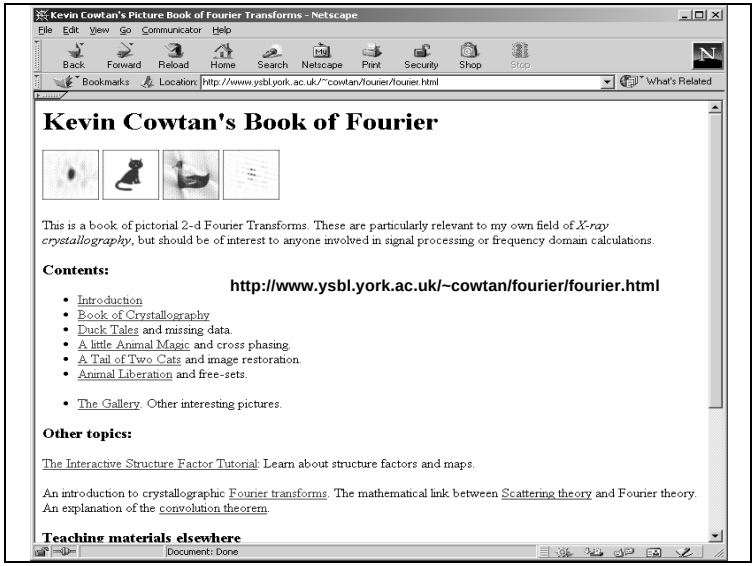
Five horizontal holes with various spacings

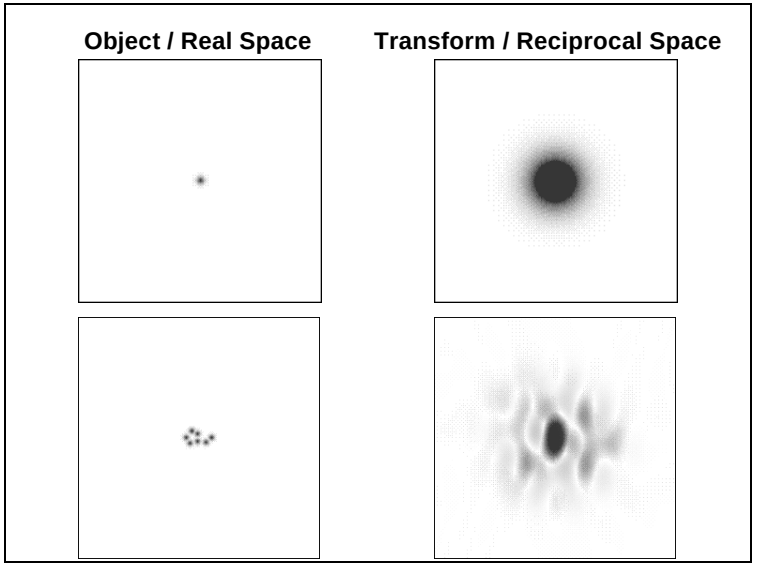


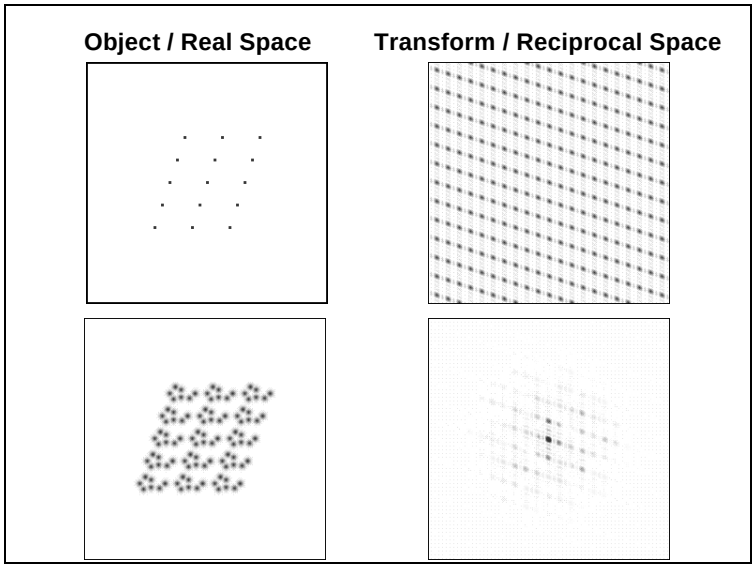
Transforms / Reciprocal Space

Vertical holes and nets of holes




Kevin Cowtan's Picture Book of Fourier Transforms - Netscape
File Edit View Go Communicator Help
Back Forward Reload Home Search Netscape Print Security Shop Stop
Bookmarks Location: http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html What's Related
Kevin Cowtan's Book of Fourier
This is a book of pictorial 2-d Fourier Transforms. These are particularly relevant to my own field of X-ray crystallography, but should be of interest to anyone involved in signal processing or frequency domain calculations.
Contents:
http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html
Introduction
Book of Crystallography
Duck Tales and missing data.
A little Animal Magic and cross phasing.
A Tail of Two Cats and image restoration.
Animal Liberation and free-sets.
The Gallery. Other interesting pictures.
Other topics:
The Interactive Structure Factor Tutorial: Learn about structure factors and maps.
An introduction to crystallographic Fourier transforms. The mathematical link between Scattering theory and Fourier theory.
An explanation of the convolution theorem.
Teaching materials elsewhere
Document: Done


Object / Real Space
Transform / Reciprocal Space


Object / Real Space
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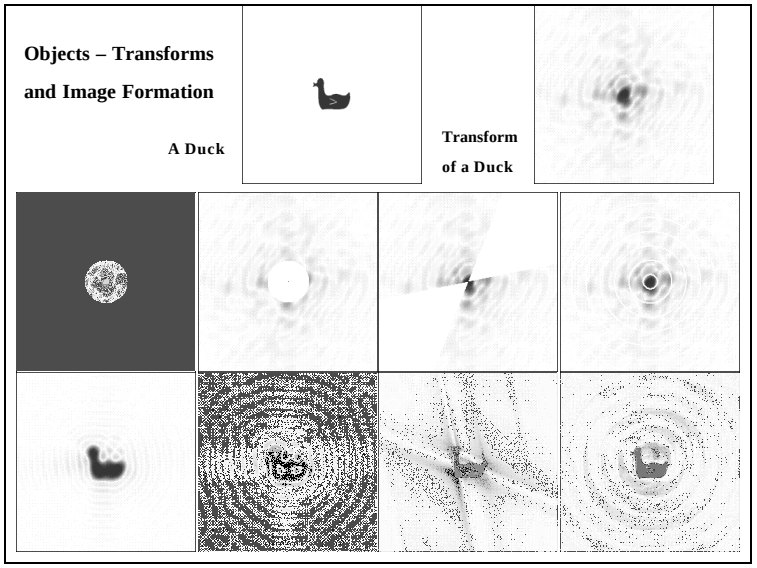
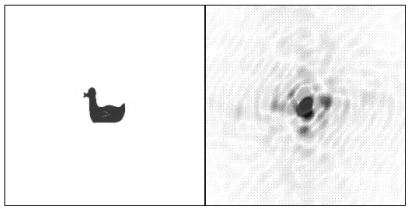

Objects – Transforms and Image Formation
A Duck
Transform of a Duck

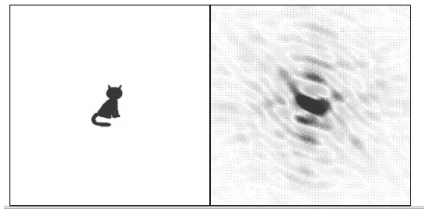
Kevin Cowtan's Book of Fourier

http://www.ysbl.york.ac.uk/~cowtan/fourier/fourier.html

Here is our old friend; the Fourier Duck, and his Fourier transform:



And here is a new friend; the Fourier Cat and *his* Fourier transform:



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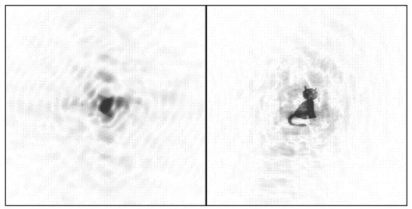
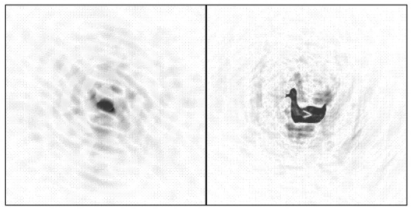
Duck Transform Amplitudes + Cat Phases



Cat Transform Amplitudes + Duck Phases



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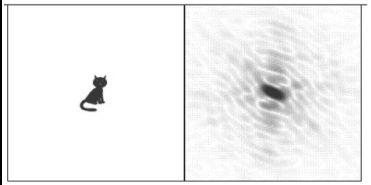
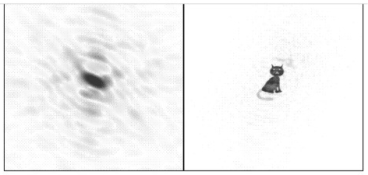
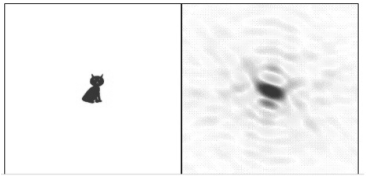
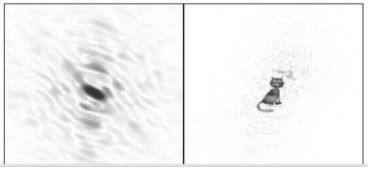


a) Cat - Cat Transform (Amplitudes only)
b) Manx (tailless) Cat - Manx Transform



c) Cat Amplitudes + Manx Phases
d) [2x(Cat Amplitudes) - Manx Amplitudes] + Manx Phases





X-Ray Crystallography

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Topics:

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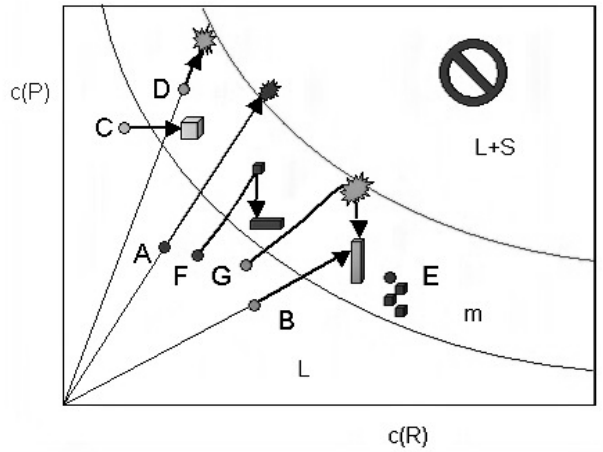
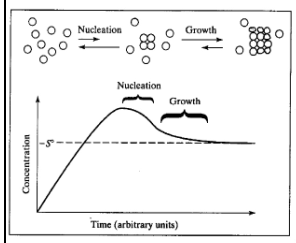
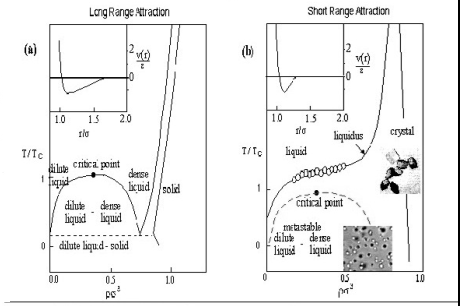
Variables that influence crystal growth

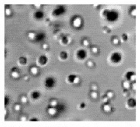
1. **Nature of macromolecule – Purity and concentration of macromolecule**
2. **Nature and concentration of precipitant**
3. **pH / Temperature / Pressure**
4. **Level of reducing agent or oxidant**
5. **Substrates, coenzymes, and ligands / Metal ions**
6. **Preparation and storage of macromolecule / Proteolysis and fragmentation**
7. **Age of macromolecule / Degree of denaturation**
8. **Vibration and sound**
9. **Volume of crystallization sample**
10. **Seeding**
11. **Amorphous precipitate**
12. **Buffers**
13. **Cleanliness**
14. **Organism or species from which the macromolecule was isolated**
15. **Gravity, gradients and convection**



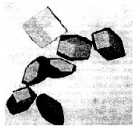
Protein Crystallization







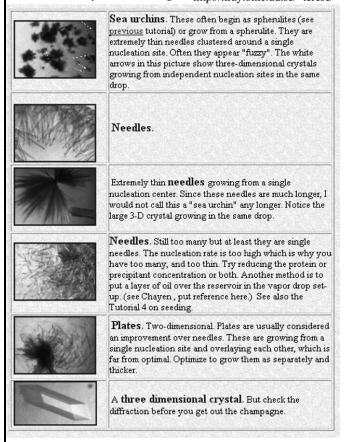
Liquid-Liquid Phase Separation
(coexistance of dilute & dense liquid)



Liquid-Crystal Phase Separation
(protein solution co-existing with protein crystal)

Types of Crystals

Welcome to the Home Page of Terese Bergfors
"The Protein Crystallization Page" http://xray.bmc.uu.se/~terese/



Sea urchins. These often begin as spherulites (see previous tutorial) or grow from a spherulite. They are extremely thin needles clustered around a single nucleation site. Often they appear "fuzzy". The white arrows in this picture show three-dimensional crystals growing from independent nucleation sites in the same drop.

Needles.

Extremely thin **needles** growing from a single nucleation center. Since these needles are much longer, I would not call this a "sea urchin" any longer. Notice the large 3-D crystal growing in the same drop.

Needles. Still too many but at least they are single needles. The nucleation rate is too high which is why you have too many, and too thin. Try reducing the protein or precipitant concentration or both. Another method is to put a layer of oil over the reservoir in the vapor drop set-up. (see Chayen, put reference here.) See also the Tutorial 4 on seeding.

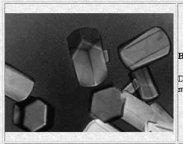
Plates. Two-dimensional. Plates are usually considered an improvement over needles. These are growing from a single nucleation site and overlaying each other, which is far from optimal. Optimize to grow them as separately and thicker.

A **three dimensional crystal**. But check the diffraction before you get out the champagne.

Welcome to the Home Page of Terese Bergfors
"The Protein Crystallization Page"
http://xray.bmc.uu.se/~terese/

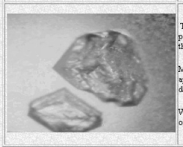
Tutorial 1. Appearances can be deceiving!

The first thing you should learn is that the appearance (habit, morphology, etc.) of your crystal is NOT what is important. Beautiful looking crystals may not diffract and really ugly crystals might diffract excellently. The only definitive proof of a "GOOD" crystal is its diffraction pattern in the X-ray beam. Therefore, do not be misled by the appearance of your crystal--mount it and check it in the beam.



Beauty is only skin deep.

Don't be fooled by appearances. These crystals may look nice, but they don't diffract.



These are ugly. In fact they are so ugly you probably wouldn't even bother to mount them but they diffract to 1.6Å.

Moral of the story: don't always go by the appearances of your crystals. It is the X-ray diffraction pattern that counts.

With that said, you can now continue the tutorial on interpreting your crystallization drop.

Common Compounds used in Crystallization

Ammonium or sodium sulfate
Sodium or ammonium citrate
Sodium or ammonium acetate
Magnesium sulfate
Cetyltrimethyl ammonium salts
Polyethylene glycol 400, 1000, 4000, 6000, 15,000 (now also 2,000, 8,000, etc.)

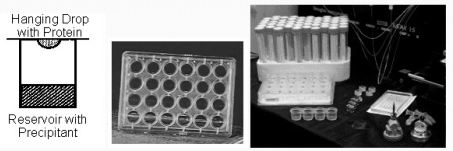
Methods for protein crystallization

Batch crystallization (simply dump reagents together)
Liquid-liquid diffusion in a capillary tube
Vapor diffusion-the most successful method (hanging drop, sitting drop), typically using a Limbro plate. Equilibration occurs between the liquid and vapor phase.
Dialysis

Hanging Drop Method - Crystal Screening

The Experimental Setup

In order to obtain a crystal, the protein molecules must assemble into a periodic lattice. One starts with a solution of the protein with a fairly high concentration (2-50 mg/ml) and adds reagents that reduce the solubility close to spontaneous precipitation. By slow further concentration, and under conditions suitable for the formation of a few nucleation sites, small crystals **may** start to grow. Often very many conditions have to be tried to succeed. This is usually done by initial screening, followed by a systematic optimization of conditions Crystals should to be a few tenth of a mm in each direction to be useful for diffraction experiments.



Right : The hanging drop technique. Center : 24 such hanging drop experiments are set up in a Linbro plate. Right : A kit of different screening solutions, a set-up Linbro plate, dialysis buttons and a micro batch plate behind a goniometer head.

The most common setup to grow protein crystals is by the **hanging drop** technique : A few microliters of protein solution are mixed with an about equal amount of reservoir solution containing the precipitants. A drop of this mixture is put on a glass slide which covers the reservoir. As the protein/precipitant mixture in the drop is less concentrated than the reservoir solution (remember: we mixed the protein solution with the reservoir solution about 1:1), water evaporates from the drop into the reservoir. As a result the concentration of both protein and precipitant in the drop slowly increases, and crystals may form. There is a variety of other techniques available such as sitting drops, dialysis buttons, and gel and microbatch techniques. Robots are useful for automatic screening and optimization of crystallization conditions. We have implemented a web computing service of Brent Segelke's CRYSTOOL, an inherently efficient random screen for crystallization conditions that you can customize. The main advantage is the small sample size a crystallization robot can handle reproducibly, but it needs some effort to set it up. Click here to learn more about the IMPAX-II robot.

Hampton Crystal Screen Solutions

Note :

A mini-screen can be set up from the most successful conditions. Those are indicated in the column labeled Miniscreen.

- a nice list of detergents commonly used in crystallization experiments.
- pretty pictures!
- CRYSTOOL efficient random screen made for you here on the WEB.

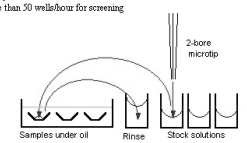
Tube #	SALT	BUFFER	Precipitant	Miniscreen	Tube #
1	0.02M Calcium Chloride	0.1M Na Acetate pH 4.6	30% w/v 2-methyl-2,4-pentanediol	Y	1
2	None	None	0.4M K,Na Tartrate tetrahydrate		2
3	None	None	0.4M Ammonium dihydrogen phosphate		3
4	None	0.1M Tris-HCl pH 8.5	2.0M Ammonium Sulfate	Y	4
5	0.2M tri-sodium citrate	0.1M Na HEPES pH 7.5	30% w/v 2-methyl-2,4-pentanediol		5
6	0.2M Magnesium chloride	0.1M Tris-HCl pH 8.5	30% w/v PEG 4000		6
7	None	0.1M Na Cacodylate pH 6.5	1.4M Sodium acetate trihydrate		7
8	0.2M tri-sodium citrate	0.1M Na Cacodylate pH 6.5	30% v/v 2-propanol		8
9	0.2M Ammonium acetate	0.1M Na Citrate pH 5.6	30% w/v PEG 4000	Y	9
10	0.2M Ammonium acetate	0.1M Na Acetate pH 4.6	30% w/v PEG 4000	Y	10
11	None	0.1M Na Citrate pH 5.6	1.0M Ammonium dihydrogen phosphate		11
12	0.2M Magnesium chloride	0.1M Na HEPES pH 7.5	30% v/v 2-propanol		12
13	0.2M tri-sodium citrate	0.1M Tris-HCl pH 8.5	30% v/v PEG 400		13
14	0.2M Calcium Chloride	0.1M Na HEPES pH 7.5	28% v/v PEG 400	Y (best)	14
15	0.2M Ammonium acetate	0.1M Na Cacodylate pH 6.5	30% w/v PEG 8000		15
16	None	0.1M Na HEPES pH 7.5	1.5M Lithium sulfate monohydrate	Y	16
17	0.2M Lithium sulfate	0.1M Tris-HCl pH 8.5	30% w/v PEG 4000	Y (2nd best)	17

Using Oryx 6 for Crystallization with Microbatch

Microbatch operation is identical to IMPAX 1-5

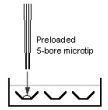
http://www.douglas.co.uk/oryx.htm

Very Fast - 240 wells/hour
more than 50 wells/hour for screening



Screening

Uses little protein
0.1 - 1 µl per well



Optimization

Microbatch screening finds more leads
than VD in a given time

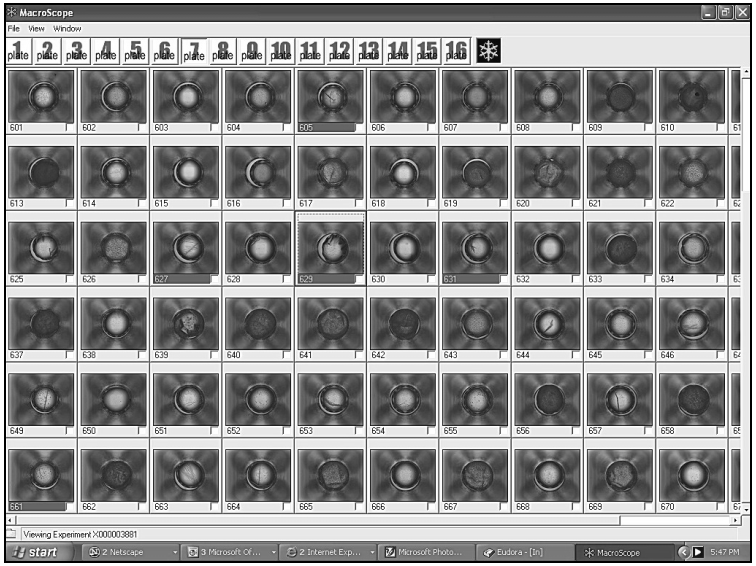
	Automated MB	Manual VD
Proteins screened	6	6
Screening solutions	48	48
Runs	3	1
Volume per well	1 + 1µl	4 +4 µl
Total protein used	864 µl	1152µl
Operator time	3 hr	24 hr
Crystallization conditions found	43	41
Unique conditions	17	15

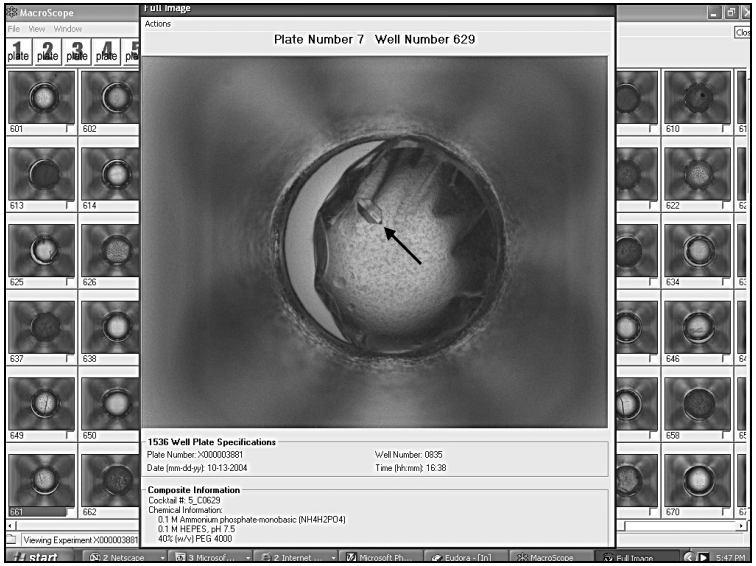
J. Crystal Growth, 168 (1996),pp 170-174. or: http://www.douglas.co.uk/tvp2.htm

Large diffracting crystals

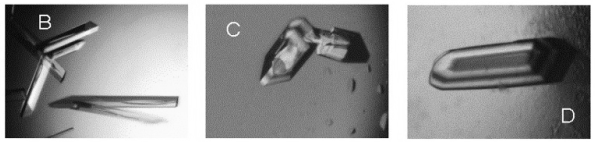
MB crystals offirdly horiferax. Data could not be collected from VD crystals which were unstable. Courtesy of E. Conti. Acta Crystallographica. D 52 (1996), pp 876-878.
http://www.douglas.co.uk/tvp3.htm

MB crystal of alcohol dehydrogenase from a thermophilic bacterium. Courtesy of Y. Korkhin. Acta Crystallographica. D 52 (1996),pp 882-886.
http://www.douglas.co.uk/tvp1.htm

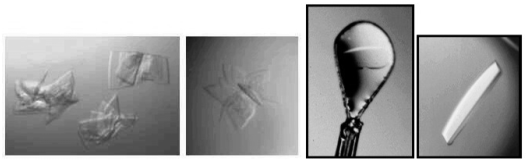




HisJ - His complex:



Tetanus Toxin C Fragment:



http://www.ccp14.ac.uk/ccp/web-mirrors/llnlrupp/crystal_lab/Crys_lab.html

X-Ray Crystallography

"If a picture is worth a thousand words, then a macromolecular structure is priceless to a physical biochemist." – van Holde text

Topics:

1. Image Formation

Resolution / Wavelength (Amplitude, Phase) / Light Microscopy / EM / X-ray / NMR

2. X-Ray Crystallography

a) Crystal Growth – Materials / Methods

b) What is a Crystal: Lattices - Lattice Constants / Space Groups / Asymmetric Unit

c) X-ray Sources – Sealed Tube / Rotation Anode / Synchrotron

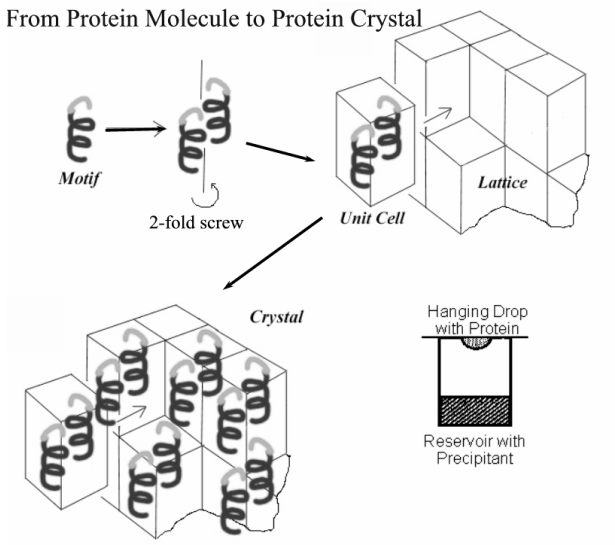
d)Theory of Diffraction – Bragg's Law / Reciprocal Space

e) Data Collection – Methods / Detectors / Structure Factors

f) Structure Solution – Phase Problem: MIR / MR / MAD

h) Refinements and Models

i) Analysis and presentation of results



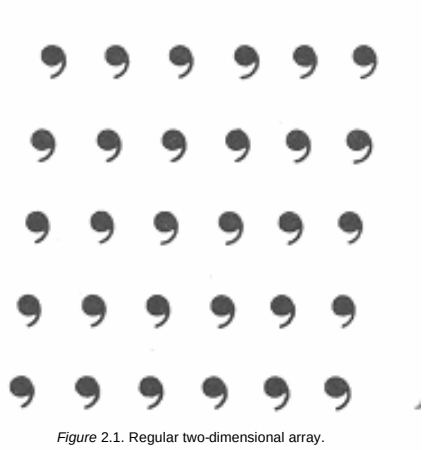


Figure 2.1. Regular two-dimensional array.

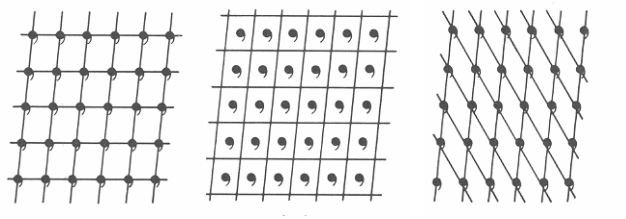


Figure 2.2. Three different grid systems referred to the array of Fig. 2.1.

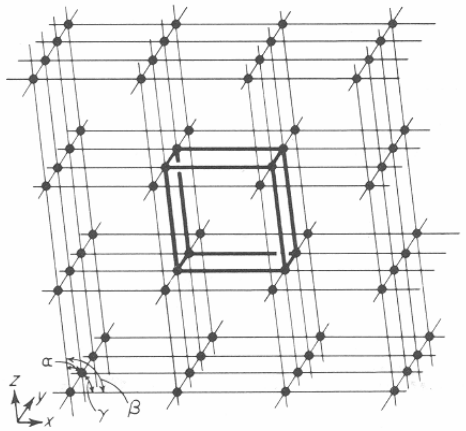


Figure 2.3. Three-dimensional lattice, showing unit cell (heavy lines).

Unit Cell Selection is Based on Symmetry

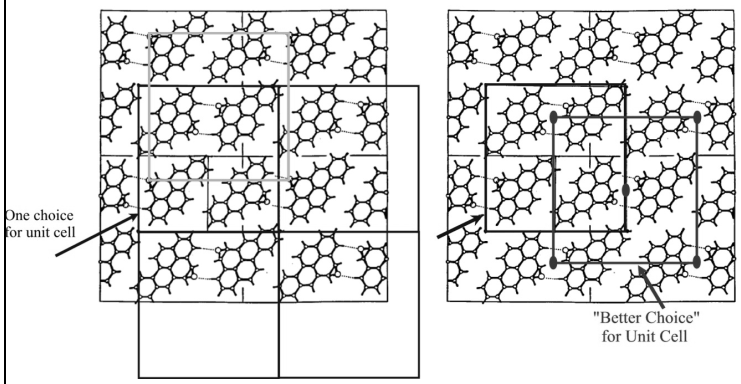
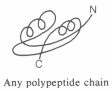
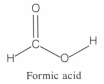
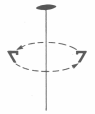
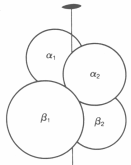
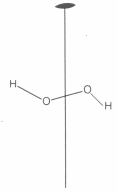
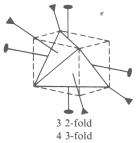
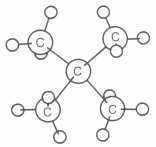
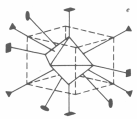
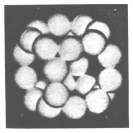


TABLE 16-1 *Examples of Cyclic Point Groups*

POINT GROUPS	H-M	NUMBER OF ASYMMETRIC UNITS	CONTACT TYPE[b]	SYMMETRY ELEMENTS	EXAMPLES[c]
C_1	1	1	none		 Any polypeptide chain  Formic acid
C_2	2	2	*i*		 Hemoglobin  Hydrogen peroxide

Examples of Cubic Point Groups

POINTS	GROUP[a] H-M	NUMBER OF ASYMMETRIC UNITS	CONTACTS[b] MAXIMUM	CONTACTS[b] MINIMUM	SYMMETRY ELEMENTS	EXAMPLES
T	23	12	*hi*	*hi*	 3 2-fold 4 3-fold	Aspartate-β-decarboxylase[c] Neopentane[d] 
O	432	24	*hii*	*hh* or *hi*	 6 2-fold 4 3-fold 3 4-fold	Dihydrolipoyl transsuccinylase[f]  Spherical subunit model  Electron density at low resolution

Crystal Systems

Crystal System	Bravais Type(s)	External Minimum Symmetry	Unit Cell Properties
Triclinic	P	None	a, b, c, al, be, ga,
Monoclinic	P, C	One 2-fold axis, parallel b (b unique)	a, b, c, 90, be, 90
Orthorhombic	P, I, F	Three perpendicular 2-folds	a, b, c, 90, 90, 90
Tetragonal	P, I	One 4-fold axis, parallel c	a, a, c, 90, 90, 90
Trigonal	P, R	One 3-fold axis	a, a, c, 90, 90, 120
Hexagonal	P	One 6-fold axis	a, a, c, 90, 90, 120
Cubic	P, F, I	Four 3-folds along space diagonal	a, a, a, 90, 90, 90

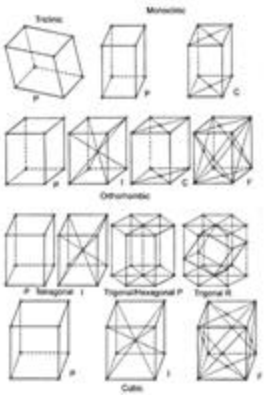
Symmetry operations: 1,2,3,4,6, -1,-2,-3,-4,-6, m

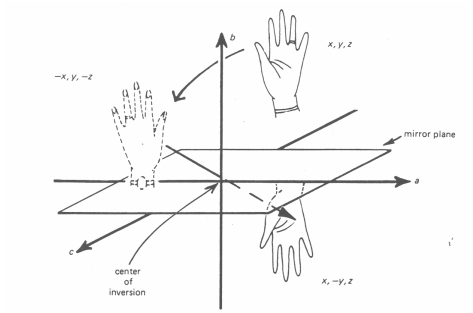
Crystal System	Point groups	Laue Class	Patterson Symmetry
Triclinic	1, -1	-1	P-1
Monoclinic	2, m, 2/m	2/m	P2/m, C2/m
Orthorhombic	222, mm2 , mmm	mmm	Pmmm, Cmmm, Fmmm, Immm
Tetragonal	4, -4, 4/m, 422, 4mm, -42m, 4/mmm	4/m, 4/mmm	P4/m, I4/m, P4/mmm, I4/mmm
Trigonal	3, -3, 32, 3m, -3 m	-3, -3m	P-3, R-3, P-3m1, P-31m, R-3m
Hexagonal	6, -6, 6/m, 622, 6mm, -62m, 6/mmm	6/m, 6/mmm	P6/m, P6/mmm
Cubic	23, m-3, 432, -43m, m3m	m-3, m-3m	Pm-3, Im-3, F-3m, Fm-3m, Fm-3m, Im-3m

Notes

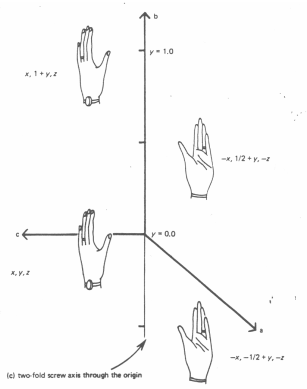
- Laue class corresponds to symmetry of reciprocal space (diffraction pattern)
- Patterson symmetry is Laue class plus allowed Bravais centering, i.e. centrosymmetric and symorphic

The 14 Bravais Lattices





(b) two-fold rotatory-inversion axis *or* mirror plane



(c) two-fold screw axis through the origin

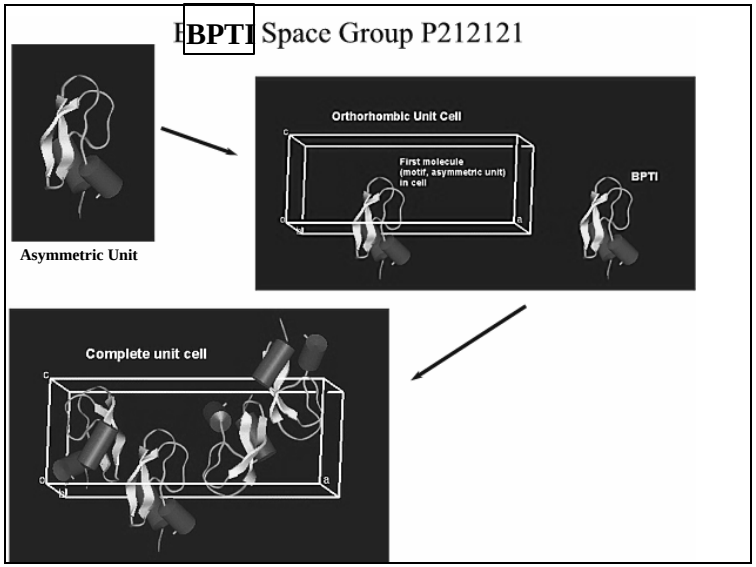
TABLE 3.4 Space Groups in Standard Orientations*

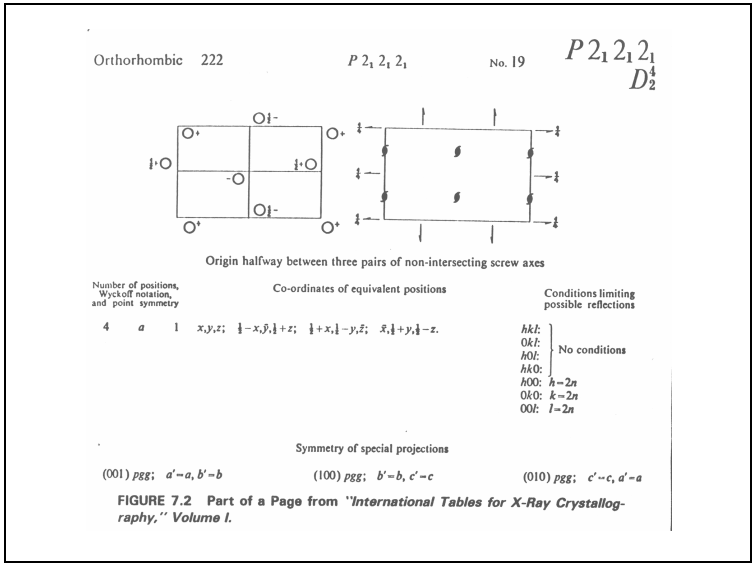
System	Point Group	Space Group						Fraction
Triclinic	1	$P1$						1/2
	$\bar{1}$	$P\bar{1}$						
Monoclinic	2	$P2$	$P2_1$	$C2$				1/4
	m	Pm	Pc	Cm	Cc			
	$2/m$	$P2/m$	$P2_1/m$	$C2/m$	$P2/c$	$P2_1/c$	$C2/c$	
Orthorhombic	222	$P222$	$P222_1$	$P2_12_12$	$P2_12_12_1$	$C222_1$	$C222$	1/8
		$F222$	$I222$	$I2_12_12_1$				
	$mm2$	$Pmm2$	$Pmc2_1$	$Pcc2$	$Pma2$	$Pca2_1$	$Pnc2$	
		$Pmn2_1$	$Pba2$	$Pna2_1$	$Pnn2$	$Cmm2$	$Cmc2_1$	
		$Ccc2$	$Amm2$	$Abm2$	$Ama2$	$Aba2$	$Fmm2$	
		$Fdd2$	$Imm2$	$Iba2$	$Ima2$			
	mmm	$Pmmm$	$Pnnn$	$Pccm$	$Pban$	$Pmma$	$Pnna$	
		$Pmna$	$Pcca$	$Pbam$	$Pccn$	$Pbcm$	$Pnnm$	
		$Pmnn$	$Pbcn$	$Pbca$	$Pnma$	$Cmcm$	$Cmca$	
		$Cmmm$	$Cccm$	$Cmma$	$Ccca$	$Fmmm$	$Fddd$	
		$Immm$	$Ibam$	$Ibca$	$Imma$			
Tetragonal	4	$P4$	$P4_1$	$P4_2$	$P4_3$	$I4$	$I4_1$	1/8
	$\bar{4}$	$P\bar{4}$	$I\bar{4}$					
	$4/m$	$P4/m$	$P4_2/m$	$P4/n$	$P4_2/n$	$I4/m$	$I4_1/a$	
	422	$P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$	1/16
		$P4_22$	$P4_22_12$	$I422$	$I4_122$			
	$4mm$	$P4mm$	$P4bm$	$P4_2cm$	$P4_2nm$	$P4cc$	$P4nc$	
		$P4_2mc$	$P4_2bc$	$I4mm$	$I4cm$	$I4_1md$	$I4_1cd$	
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$	$P\bar{4}m2$	$P\bar{4}c2$	
		$P\bar{4}b2$	$P\bar{4}n2$	$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$	
	$4/mmm$	$P4/mmm$	$P4/mcc$	$P4/nbm$	$P4/nnc$	$P4/mbm$	$P4/mnc$	
		$P4/nmm$	$P4/ncc$	$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$	
		$P4_2/mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$	$I4/mmm$	$I4/mcm$	
		$I4_1/amd$	$I4_1/acd$					
Trigonal/rhombohedral	3	$P3$	$P3_1$	$P3_2$	$R3$			1/6
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$					
	32	$P312$	$P321$	$P3_112$	$P3_121$	$P3_212$	$P3_221$	1/12
		$R32$						
	$3m$	$P3m1$	$P31m$	$P3c1$	$P31c$	$R3m$	$R3c$	
	$\bar{3}m$	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$	$R\bar{3}m$	$R\bar{3}c$	
Hexagonal	6	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$	1/12
	$\bar{6}$	$P\bar{6}$						
	$6/m$	$P6/m$	$P6_3/m$					
	622	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$	1/24
	$6mm$	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$			
	$\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$			
	$6/mmm$	$P6/mmm$	$P6/mcc$	$P6_3/mcm$	$P6_3/mmc$			
Cubic	23	$P23$	$F23$	$I23$	$P2_13$	$I2_13$		1/24
	$m3$	$Pm3$	$Pn3$	$Fm3$	$Fd3$	$Im3$	$Pa3$	
		$Ia3$						
	432	$P432$	$P4_232$	$F432$	$F4_132$	$I432$	$P4_332$	1/48
		$P4_132$	$I4_132$					
	$\bar{4}3m$	$P\bar{4}3m$	$F\bar{4}3m$	$I\bar{4}3m$	$P\bar{4}3n$	$F\bar{4}3c$	$I\bar{4}3d$	
	$m3m$	$Pm3m$	$Pn3n$	$Pm3n$	$Pn3m$	$Fm3m$	$Fm3c$	
		$Fd3m$	$Fd3c$	$Im3m$	$Ia3d$			

*The 11 Laue symmetries are separated by horizontal lines.

TABLE 16-5 *The 65 "Biological" Space Groups*

CRYSTAL SYSTEM	LATTICE	MINIMUM SYMMETRY OF UNIT CELL	UNIT CELL EDGES AND ANGLES*	DIFFRACTION PATTERN SYMMETRY*	SPACE GROUPS*
Triclinic	P	None	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	$\bar{1}$	$P1$
Monoclinic	P	2-fold axis parallel to b	$a \neq b \neq c$	$2/m$	$P2$, $P2_1$
	C		$\alpha = \gamma = 90°$ $\beta \neq 90°$		$C2$
Orthorhombic	P	3 mutually perpendicular 2-fold axes	$a \neq b \neq c$	mmm	$P222$, $P2_12_12$, $P222_1$, $P2_12_12_1$
	C		$\alpha = \beta = \gamma = 90°$		$C222$, $C222_1$
	I				$I222$, $I2_12_12_1$
	F				$F222$
Tetragonal	P	4-fold axis parallel to c	$a = b \neq c$	$4/m$	$P4$, ($P4_1$, $P4_3$), $P4_2$
	I		$\alpha = \beta = \gamma = 90°$		$I4$, $I4_1$
				$4/mmm$	$P422$, ($P4_222$, $P4_122$), $P4_222$
					$P42_12$, ($P4_12_12$, $P4_32_12$), $P4_22_12$
					$I422$, $I4_122$
Trigonal/rhombohedral	$R^\dagger$	3-fold axis parallel to c	$a = b = c$	$\bar{3}$	$R3$
	$P^\dagger$		$\alpha = \beta = \gamma \neq 90°$		$P3$, ($P3_1$, $P3_2$)
				$\bar{3}m$	$R32$
					[$P321$, $P312$]
					[($P3_121$, $P3_221$), ($P3_112$, $P3_212$)]
Hexagonal	P	6-fold axis parallel to c	$a = b \neq c$	$6/m$	$P6$, ($P6_1$, $P6_5$)
			$\alpha = \beta = 90°$		$P6_3$, ($P6_2$, $P6_4$)
			$\gamma = 120°$	$6/mmm$	$P622$, ($P6_122$, $P6_522$)
					$P6_322$, ($P6_222$, $P6_422$)
Cubic	P	3-fold axes along cube diagonals	$a = b = c$	$m3$	$P23$
			$\alpha = \beta = \gamma = 90°$		$P2_13$
	I				[$I23$, $I2_13$]
	F				$F23$
				$m3m$	$P432$, ($P4_232$, $P4_332$)
					$P4_232$
					$I432$, $I4_132$
					$F432$, $F4_132$





Orthorhombic 222 $P\,2_1\,2_1\,2_1$ No. 19 $P\,2_1\,2_1\,2_1$ D_2^4

Origin halfway between three pairs of non-intersecting screw axes

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
4	*a*	1	x,y,z; $\frac{1}{2}-x,\bar{y},\frac{1}{2}+z$; $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$.	*hkl*: No conditions 0*kl*: No conditions *h*0*l*: No conditions *hk*0: No conditions *h*00: $h=2n$ 0*k*0: $k=2n$ 00*l*: $l=2n$

Symmetry of special projections

(001) *pgg*; $a'=a, b'=b$ (100) *pgg*; $b'=b, c'=c$ (010) *pgg*; $c'=c, a'=a$

FIGURE 7.2 Part of a Page from *"International Tables for X-Ray Crystallography," Volume I.*

X-Ray Crystallography

"If a picture is worth a thousand words, then a macromolecular structure is priceless to a physical biochemist." – van Holde text

Topics:

1. Image Formation

Resolution / Wavelength (Amplitude, Phase) / Light Microscopy / EM / X-ray / NMR

2. X-Ray Crystallography

a) Crystal Growth – Materials / Methods

b) Crystal Lattices - Lattice Constants / Space Groups

c) X-ray Sources – Sealed Tube / Rotation Anode / Synchrotron

d)Theory of Diffraction – Bragg's Law / Reciprocal Space

e) Data Collection – Methods / Detectors / Structure Factors

f) Structure Solution – Phase Problem: MIR / MR / MAD

h) Refinements and Models

i) Analysis and presentation of results