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. Image Formation ***(optical illusions)***

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

2. Protein Data Bank (PDB)

Data mining and Protein Structure Analysis Tools

---

3. X-Ray Crystallography

a) 100 years of X-ray Crystallography

b) Crystal Growth – Materials / Methods

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

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

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

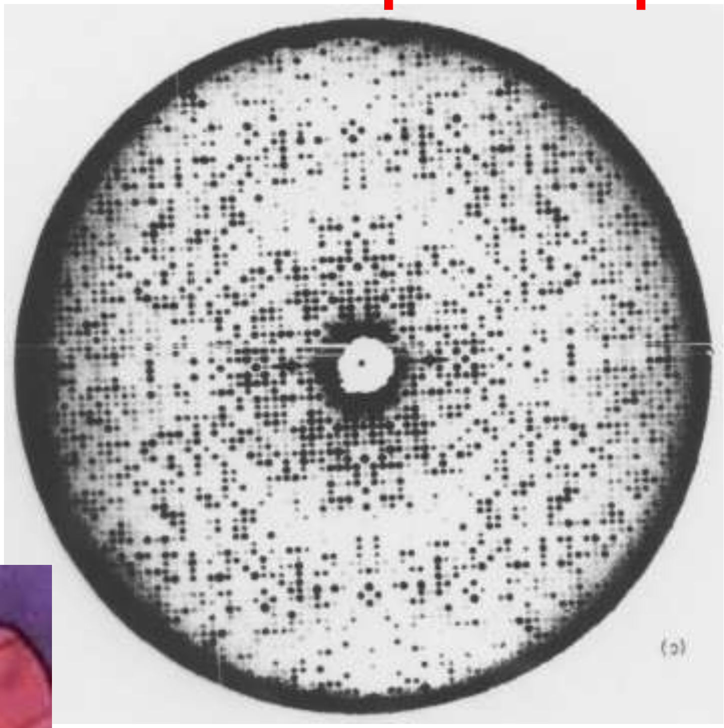
f) Data Collection – Methods / Detectors / Structure Factors

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

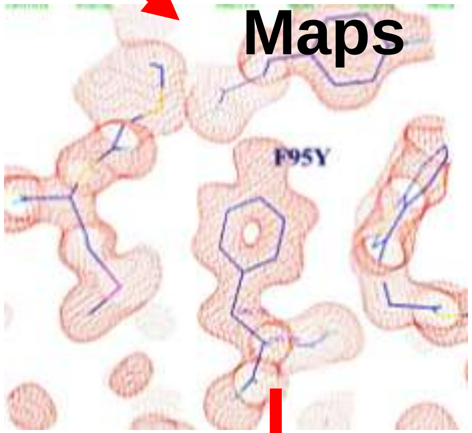
h) Refinements and Models / Analysis and presentation of results

Object → Transform → Image

Transform / Reciprocal Space

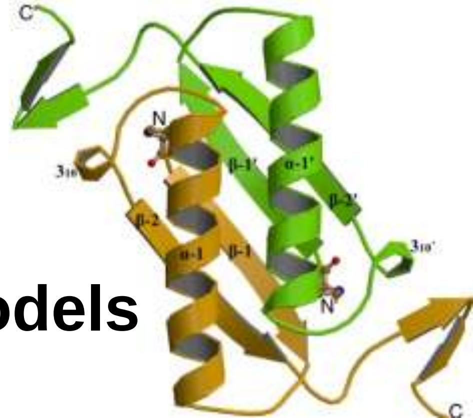


Electron Density Maps



Object / Real Space

Models



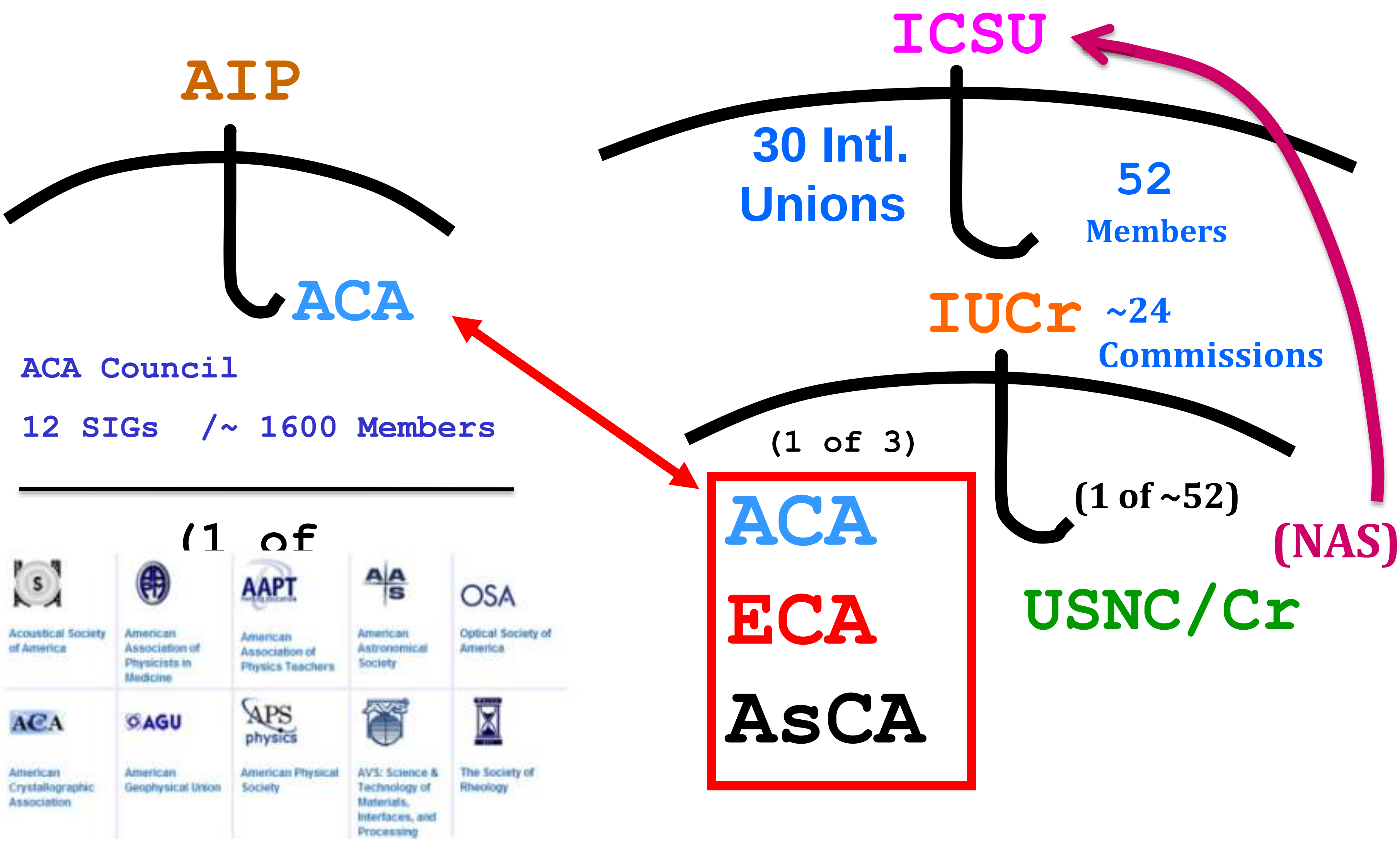
IYCr 2014

Marv Hackert - UT Austin - Fall 2013

http://www.theguardian.com/science/video/2013/oct/09/100-years-x-ray-crystallography-video-animation

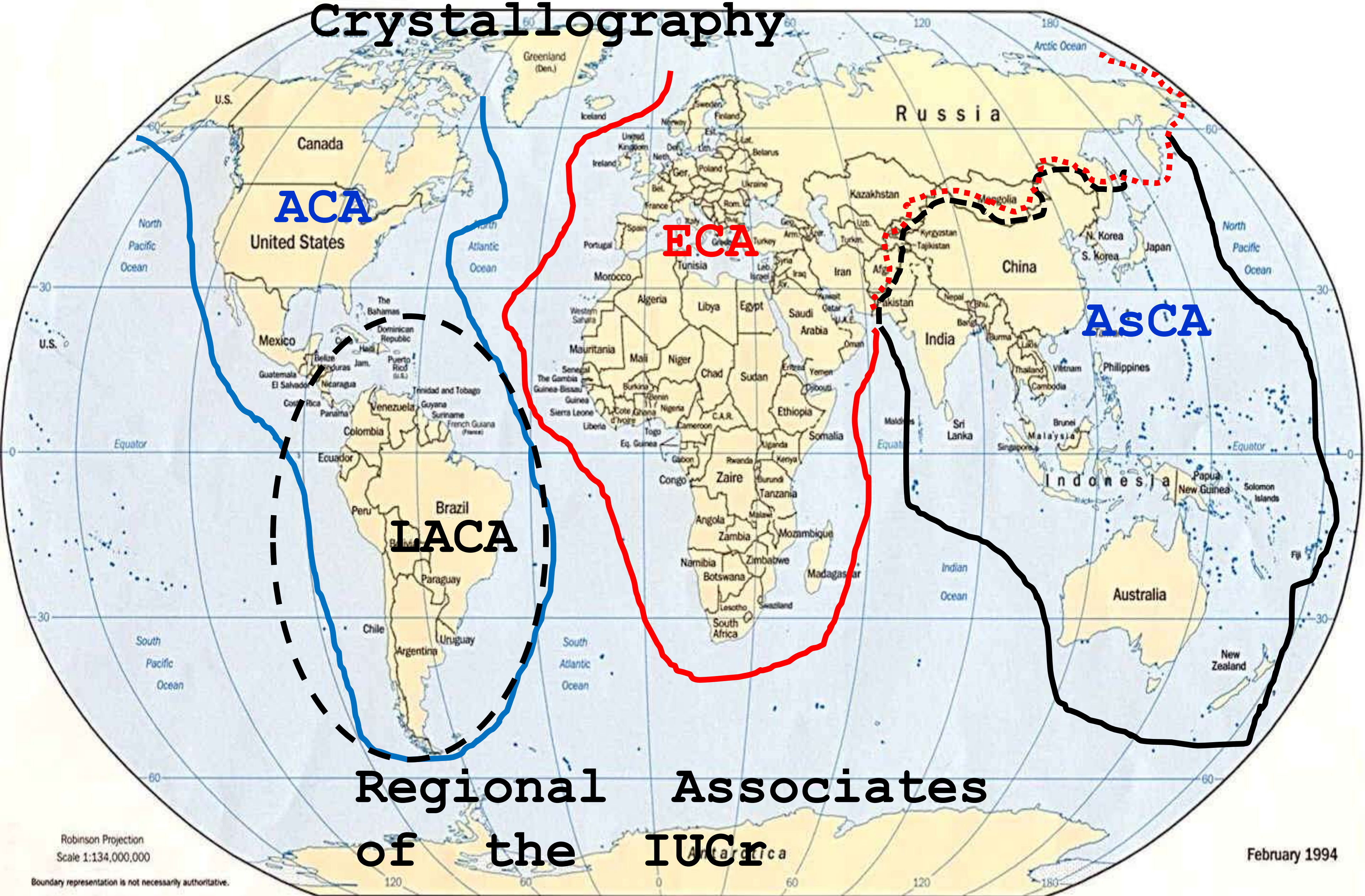
Relational Chart

ACA / AIP / USNCCr / IUCr / ICSU



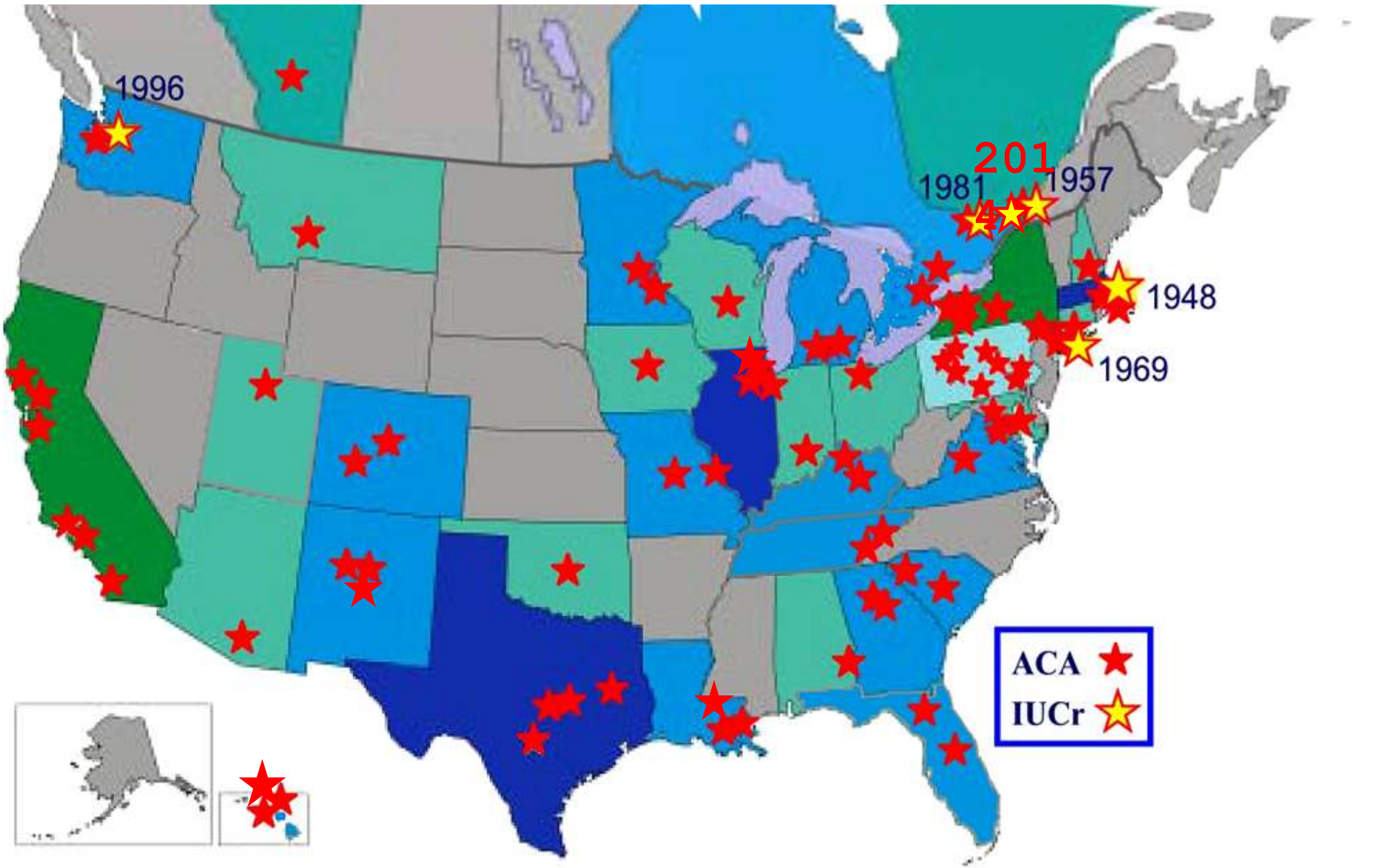
Countries that adhere to the IUCr are shown in red (43 Adhering Bodies of the IUCr, representing 52 countries, and its three Regional Associates).

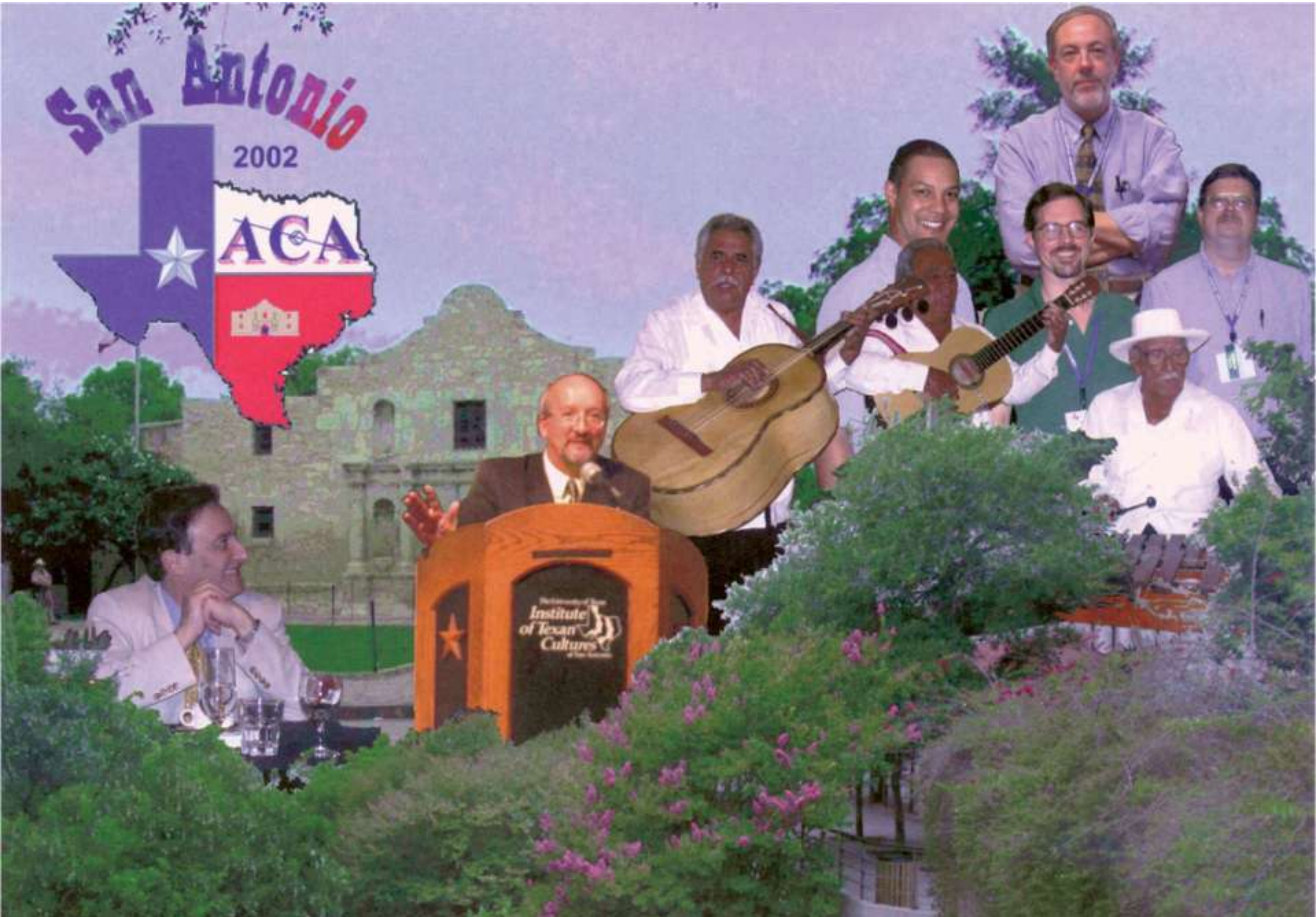
The World of Crystallography



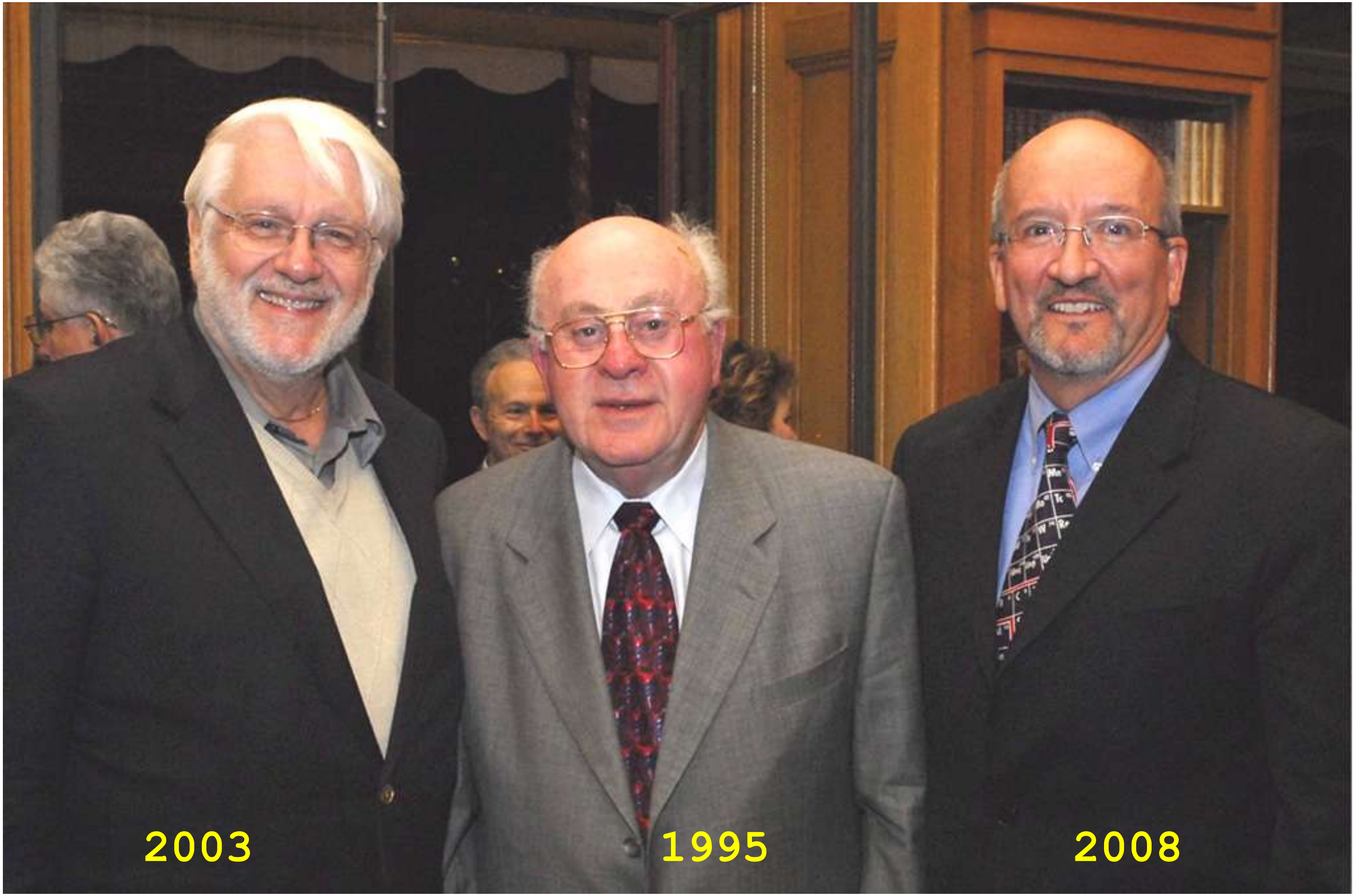
Regional Associates of the IUCr

American Crystallographic Assn.



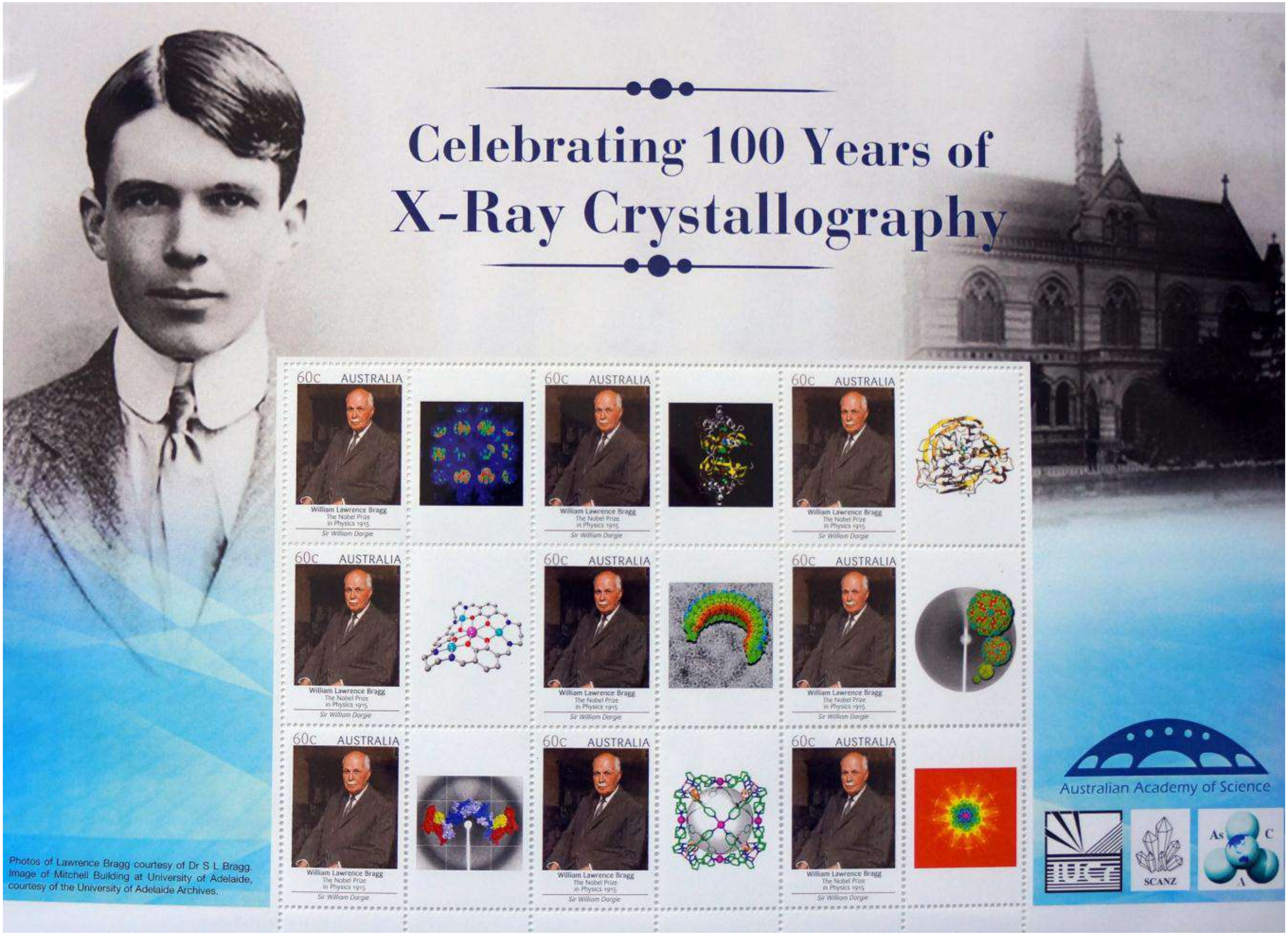

San Antonio
2002
ACA
Institute of Texan Cultures

University of Texas at Austin – ACA Presidents



***Front Row**: Elena Boldyreva, Claude Lecomte, Gautam Desiraju, Luc Van Meervelt, Sine Larsen; **Back Row:** Wulf Depmeier, Michael Dacombe, Hanna Dabkowska, Marvin Hackert, Mitchell Guss, Manuel Perez-Mato*.

Bragg Symposium: Celebrating 100 years of X-ray crystallography - *The University of Adelaide, 6th December 2012*



Celebrating 100 Years of
X-Ray Crystallography
60c AUSTRALIA
William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie
60c AUSTRALIA
William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie
60c AUSTRALIA
William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie
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William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie
60c AUSTRALIA
William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie
Australian Academy of Science
Photos of Lawrence Bragg courtesy of Dr S L Bragg.
Image of Mitchell Building at University of Adelaide,
courtesy of the University of Adelaide Archives.


opening ceremony
unesco building
paris
20-21 january 2014


IYCr2014 Opening Ceremony
ADMISSION TICKET
Paris – UNESCO Headquarters –
Room 1
7 Place de Fontenoy, 75007 Paris
20-21 January 2014

home about events contribute learn opening ceremony

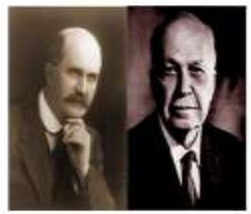
2014 international year of

Use of X-rays to determine crystal structure

Nobel Prize in Physics 1915

Sir William Henry Bragg and Sir William Lawrence Bragg

for their services in the analysis of crystal structure by means of X-rays



More... W.H. Bragg | W.L. Bragg

Timelines of Crystallography

This page initially shows a timeline of Nobel Prizes awarded for work involving cryst... ...ue was awarded the Physics Prize for the discovery of the diffraction of X-rays by crystals. Other timelines can be viewed in parallel: click on the names of those you wish to see. E... ...ghlight specific entries.

Nobel Prizes involving crystallography | Geometric crystallography | Physical crystallography | Chemical crystallography

Filter: Highlight:

Select a date or drag the timelines.

1500	1600	1700	1750
1800	1850	1900	1950
1975	2000	2010	2014

Discovery of X-rays
Use of X-rays to determine crystal structure
The wave nature of the electron
Diffraction of
Discovery of the characteristic Röntgen radiation of the elements
Dipole moments ar
Diffraction of X-rays by crystals

Get to know the Nobel Laureates! Nobelprize.org

1870 1880 1890 1900 1910 1920 1930

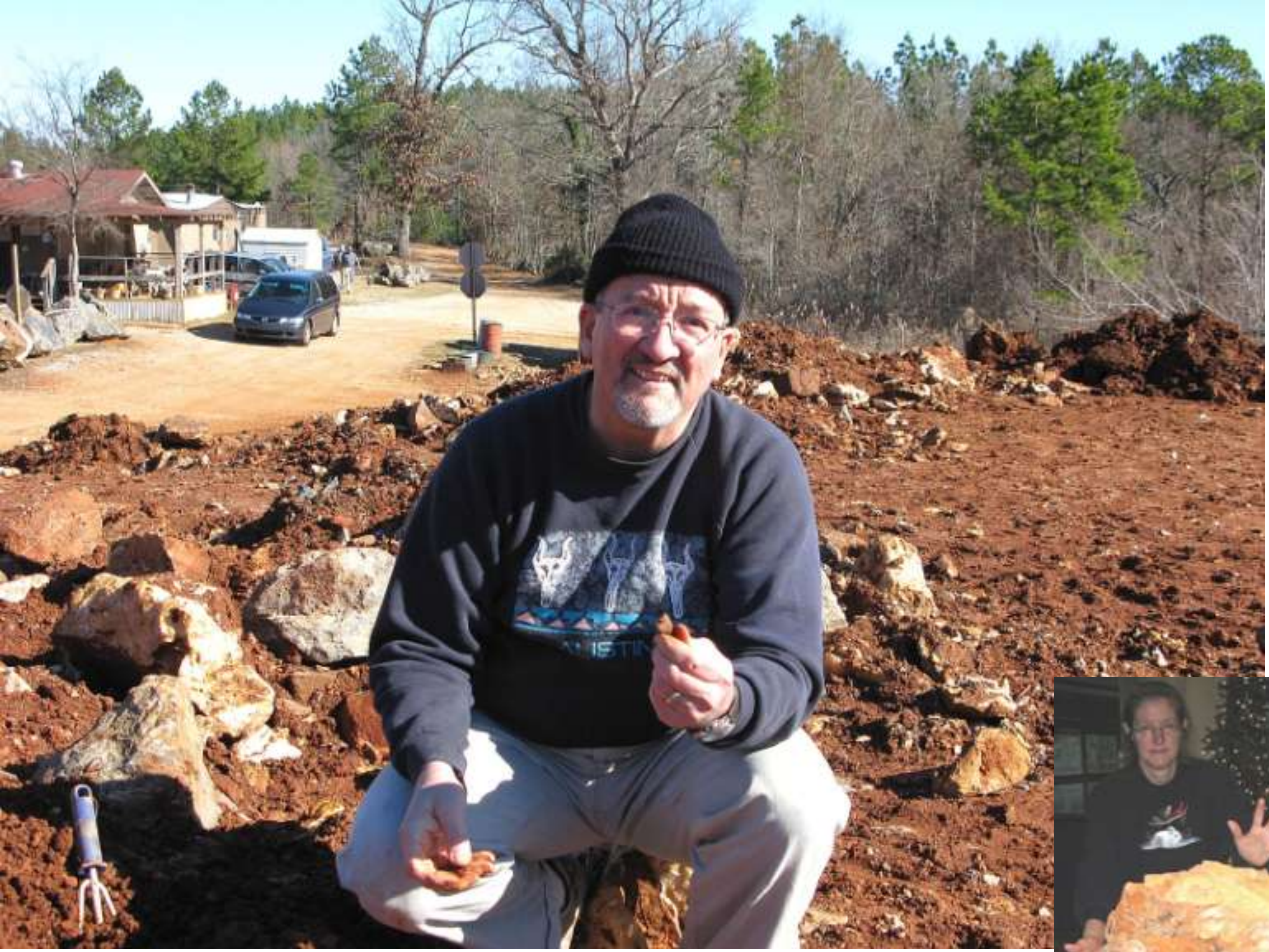
Theory of diamagnetism
Theory of ionic crystals
Studies on dislocations
Ferroelectric experiments
Diffusion in solids and defects
Zone the
nescence of crystals under X-rays
First important work on dislocations
Berek compensator
Piezoelectric resonator
Schottky
Phosphorescence of zinc sulfide under X-rays
Beginning of lattice-dynamic theory
Generation of ultrasonic waves by piezoelectric crystals
Magnetic
Phosphorescence of zinc sulfide under X-rays
Metamict minerals give no X-ray diffraction pattern
Experiments on f
ts by interferometry
Studies of edge
Concept of edge dislocati

1905 1910 1915 1920 1925

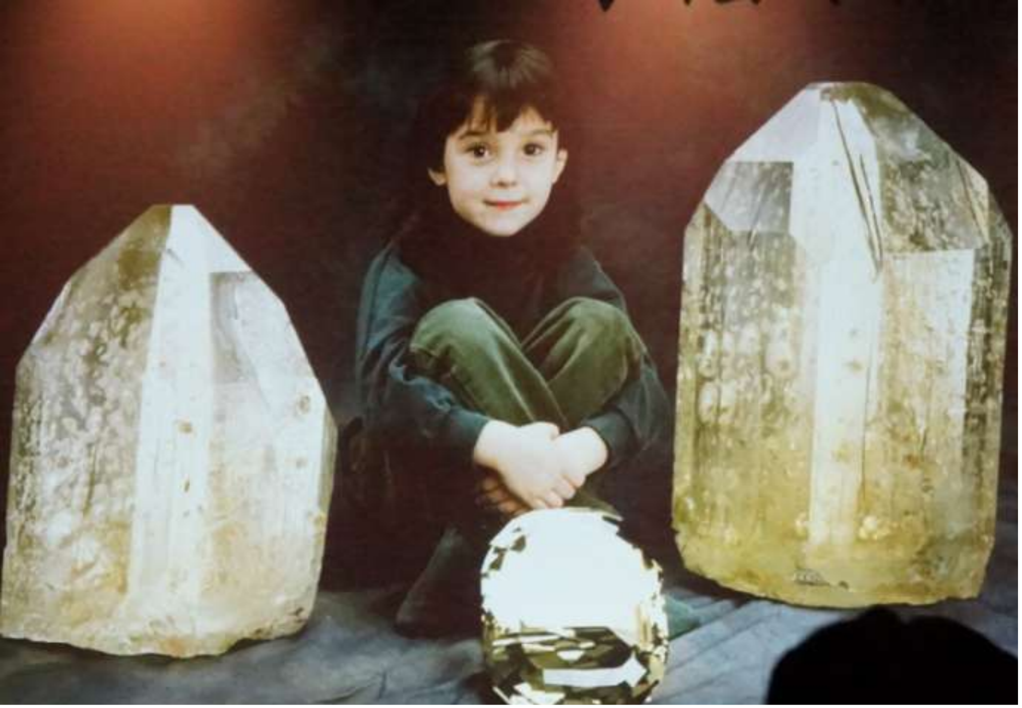
Reciprocal lattice
Spinel structures
Determination of unit-cell content
Reinvention of powder photographs
Geometrical interpretation of Bra
First structure determination
Powder photographs
Reflection powers
Corrected intensities
Fourier series to represent electron density
Friedel law
Integrated reflections; X-ray scattering by imperfect crystals
Tabulation
Contribution to the interpretation of X-ray diffraction patterns
Extinctions and space groups; graphical and analytical description of spac
Experiments on X-ray diffraction
Theory of X-ray diffraction
Primary and

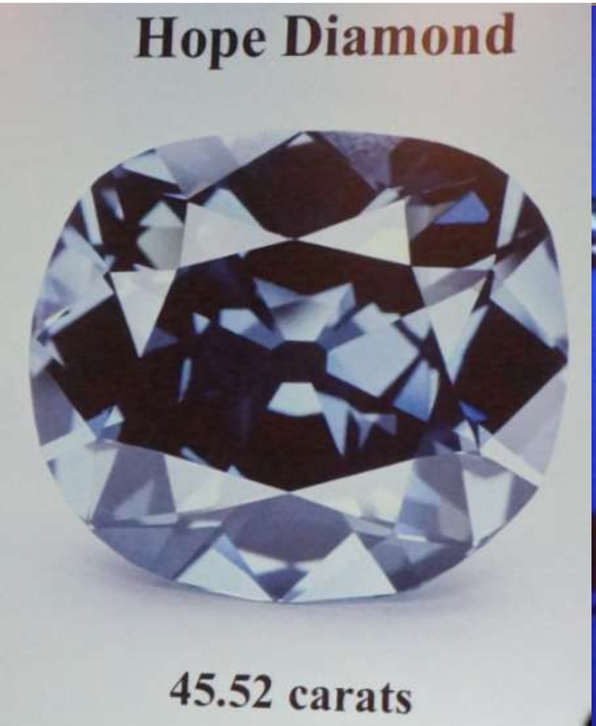
1920


...dramatic.
0 8616-28622-3 6
FOX VIDEO
NO HIGHWAY IN THE SKY
JAMES STEWART
MARLENE DIETRICH
NO HIGHWAY IN THE SKY
JAMES STEWART MARLENE DIETRICH
NO HIGHWAY IN THE SKY
Directed by HENRY KOSTER
NOT RATED



Crystallography: 1) the branch of science dealing with the formation and properties of crystals, 2) the science of condensed matter with emphasis on the atomic or molecular structure and its relation to physical and chemical properties



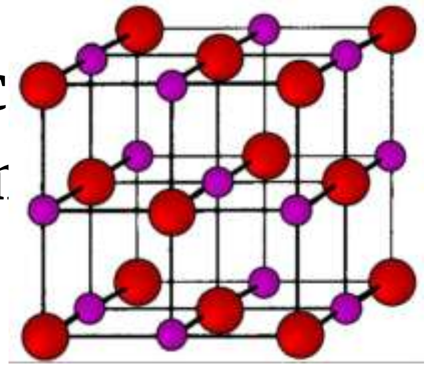

Hope Diamond
45.52 carats

Niaca Mine, Chihuahua, Mexico

X-ray diffraction

1912 Max von Laue discovered X-ray diffraction by crystals when he and his assistants directed a beam of X-rays at a crystal of copper sulfate and record the diffraction pattern on a piece of film.

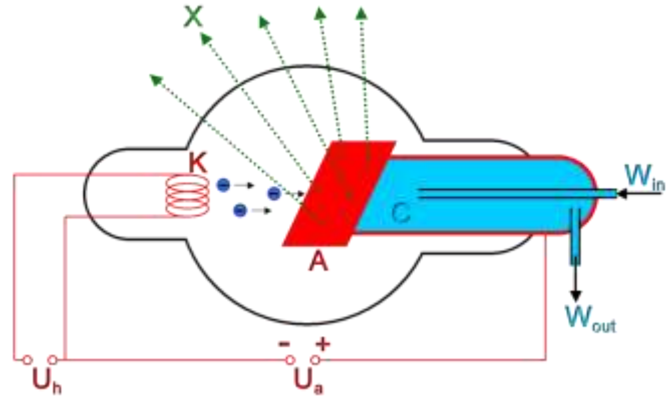
1913 W.L. Bragg reported the first c structure, the structure of Sodium



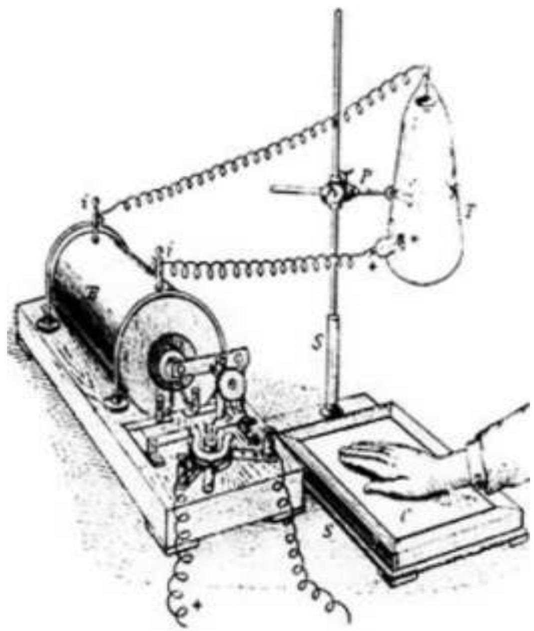
Sodium Chloride (NaCl)

The Nobel Prize in Physics 1901
Wilhelm Conrad Röntgen

The Nobel Prize in Physics 1901

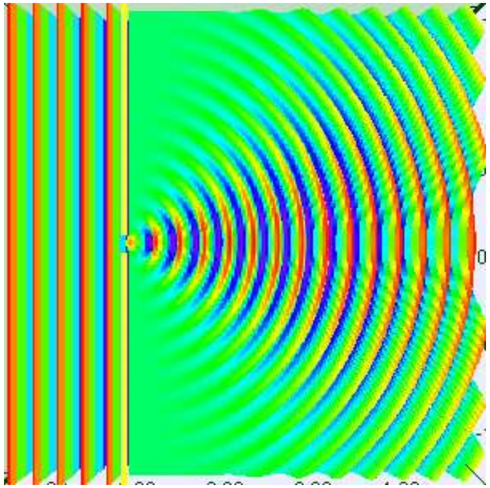


Wilhelm Conrad Röntgen

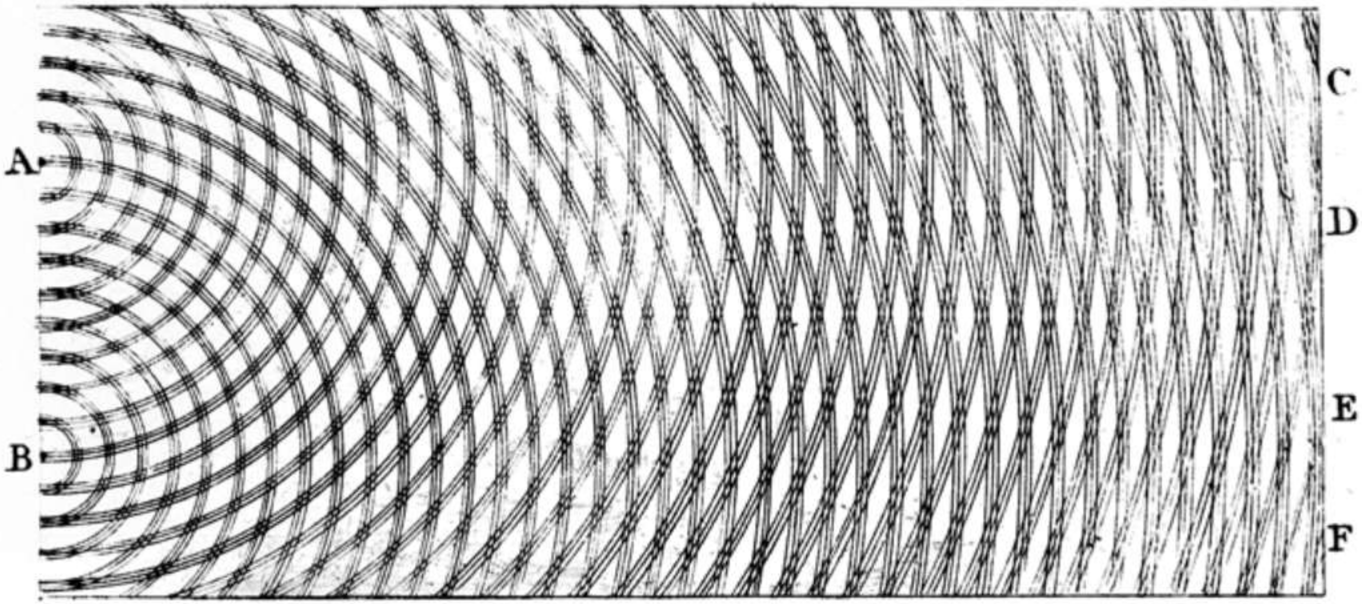


The Nobel Prize in Physics 1901 was awarded to Wilhelm Conrad Röntgen *"in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him".*

Diffraction

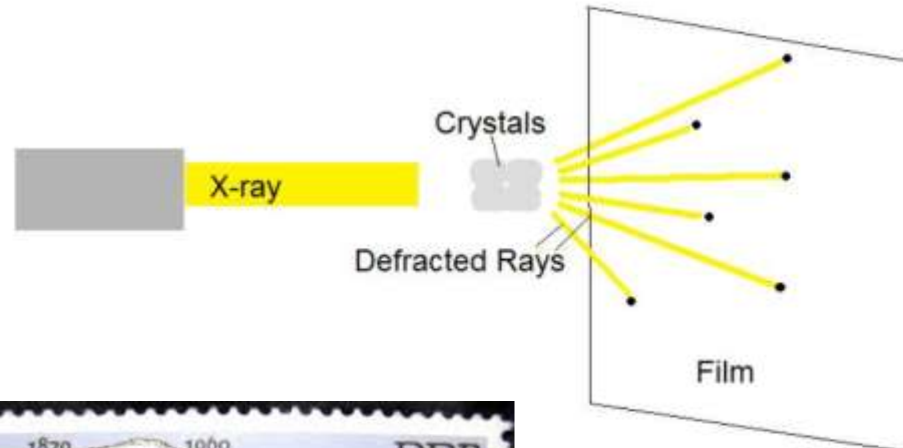


Approximation of diffraction pattern from a slit of width equal to wavelength of an incident plane wave in 3D spectrum visualization.



Thomas Young's sketch of two-slit diffraction, which he presented to the Royal Society in 1803

The Nobel Prize in Physics 1914

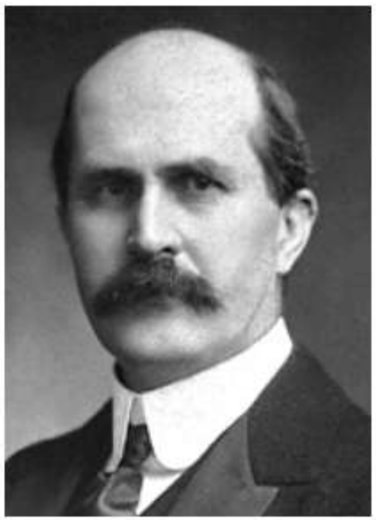


Max von Laue

The Nobel Prize in Physics 1914 was awarded to Max von Laue *"for his discovery of the diffraction of X-rays by crystals"*.

The Nobel Prize in Physics 1915
William Bragg, Lawrence Bragg

The Nobel Prize in Physics 1915

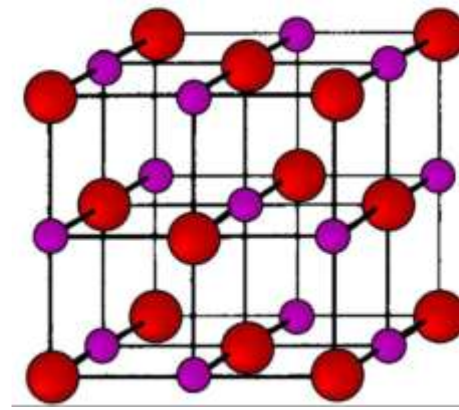


Sir William Henry Bragg

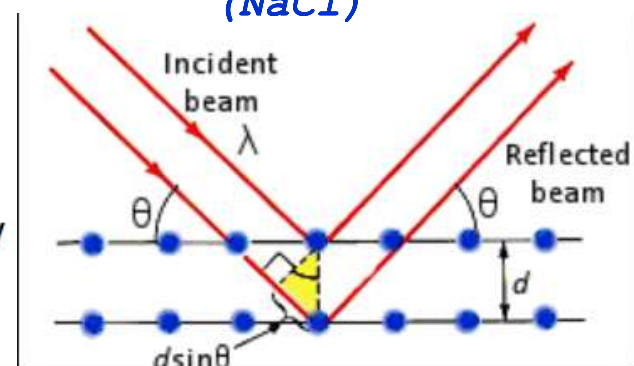
William Lawrence Bragg

The Nobel Prize in Physics 1915 was awarded jointly to Sir William Henry Bragg and William Lawrence Bragg *"for their services in the analysis of crystal structure by means of X-rays"*

X-ray apparatus



Sodium Chloride (NaCl)

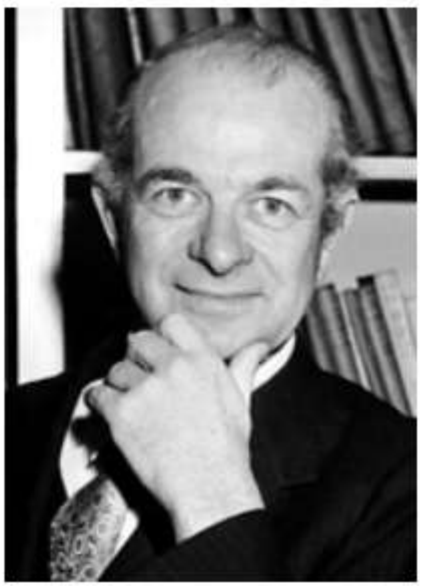


Bragg's Law ($n\lambda = 2d\sin\theta$)

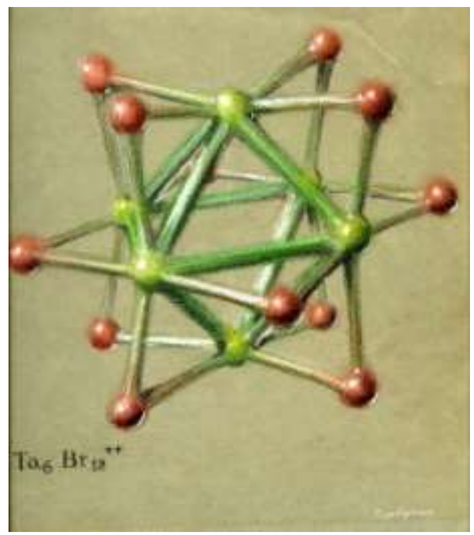
The Nobel Prize in Chemistry 1954
Linus Pauling

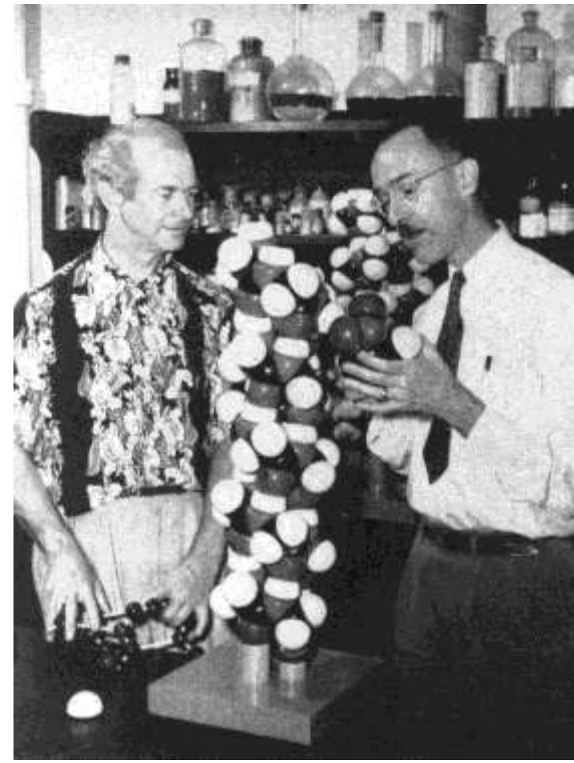
2014 international year of crystallography

The Nobel Prize in Chemistry 1954



Linus Carl Pauling





Linus Pauling & Roger Hayward

The Nobel Prize in Chemistry 1954 was awarded to Linus Pauling *"for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances"*.

The Nobel Prize in Chemistry 1962
Max F. Perutz, John C. Kendrew

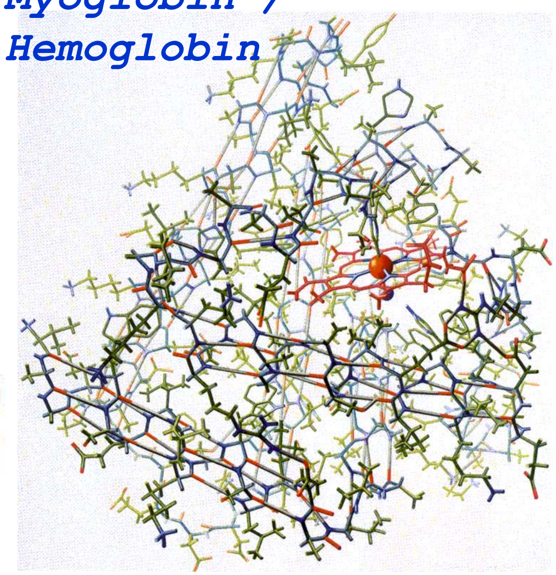
The Nobel Prize in Chemistry 1962

Max Ferdinand Perutz

John Cowdery Kendrew

The Nobel Prize in Chemistry 1962 was awarded jointly to Max Ferdinand Perutz and John Cowdery Kendrew *"for their studies of the structures of globular proteins"*

Myoglobin / Hemoglobin



The Nobel Prize in Physiology or Medicine 1962
Francis Crick, James Watson, Maurice Wilkins

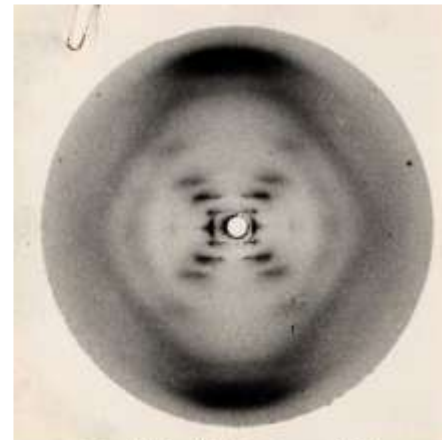
The Nobel Prize in Physiology or Medicine 1962

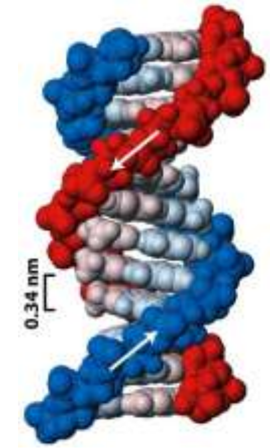

Francis Harry Compton Crick

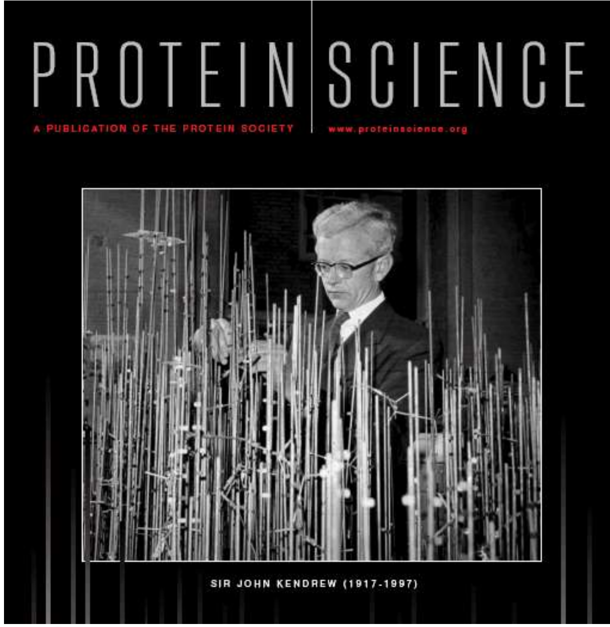

James Dewey Watson


Maurice Hugh Frederick Wilkins

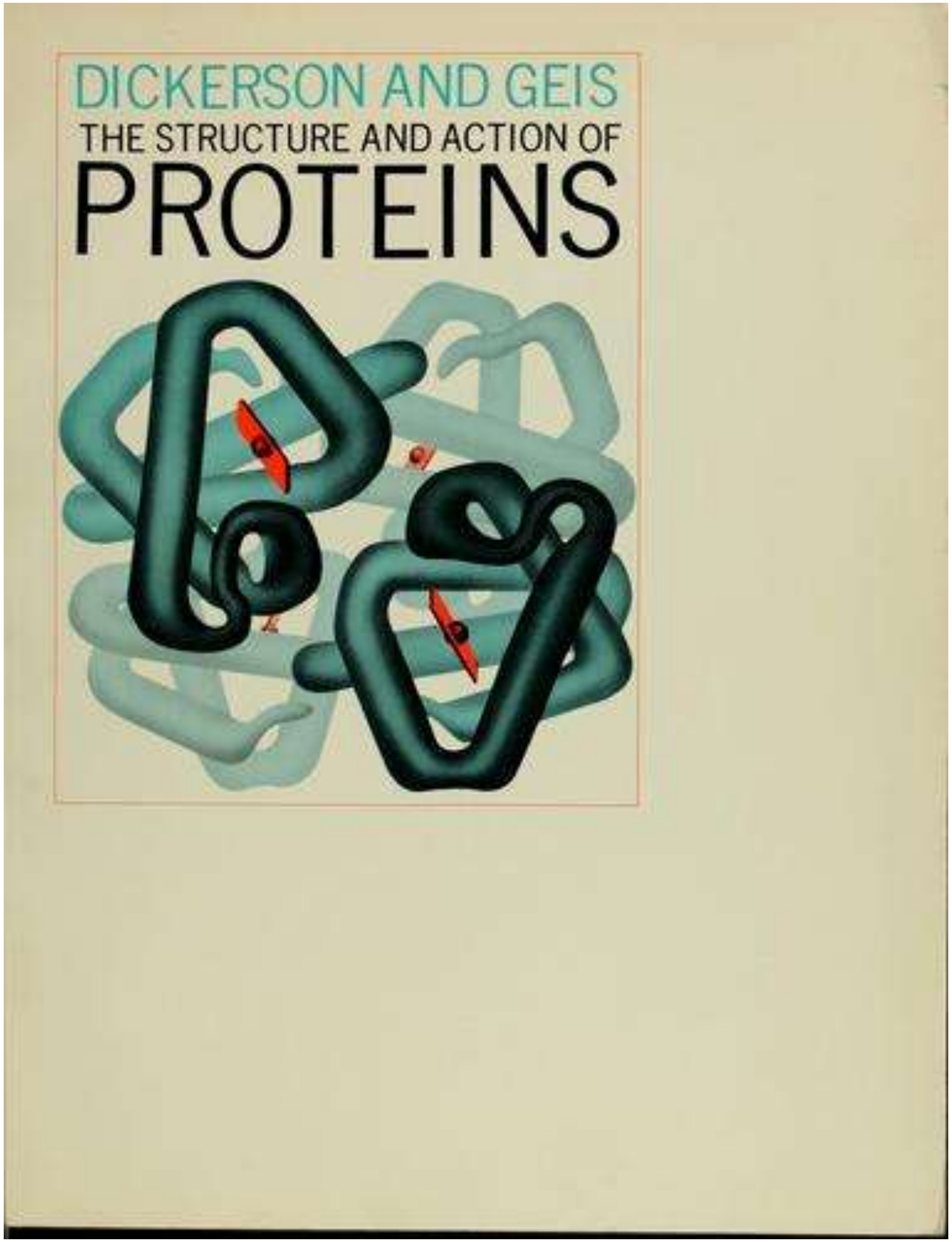
The Nobel Prize in Physiology or Medicine 1962 was awarded jointly to Francis Harry Compton Crick, James Dewey Watson and Maurice Hugh Frederick Wilkins *"for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material".*

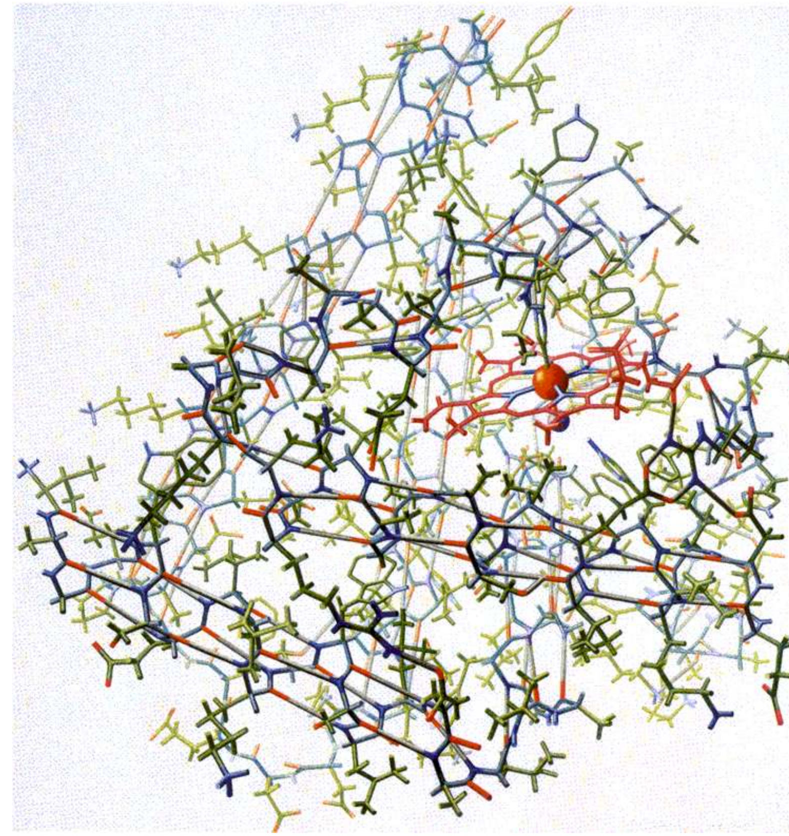

Rosalind Franklin's X-ray image of DNA





John Kendrew and his "Frankendrew Monster" at 6Å resolution

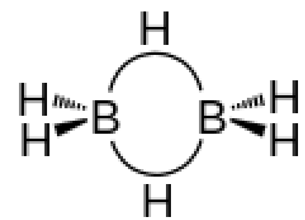

DICKERSON AND GEIS
THE STRUCTURE AND ACTION OF
PROTEINS



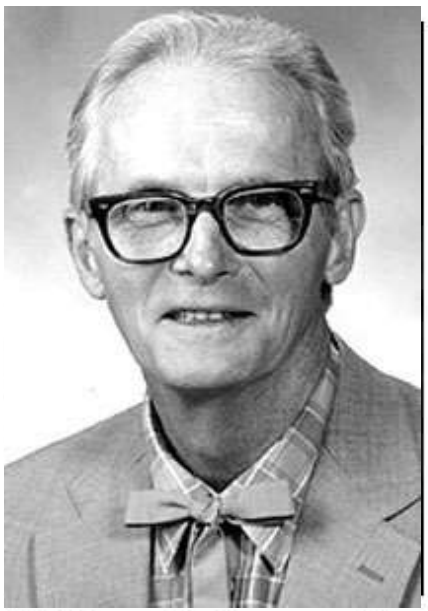
The Nobel Prize in Chemistry 1976
William Lipscomb

international year of crystallography
2014
IUCr

The Nobel Prize in Chemistry 1976



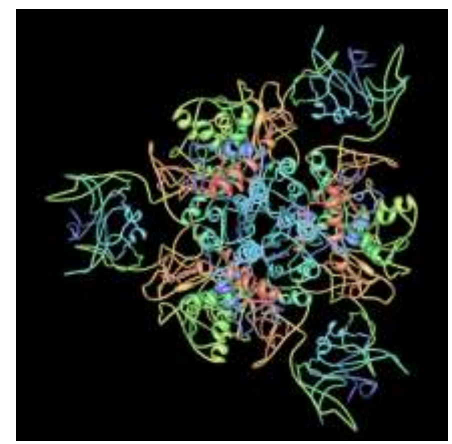
Bonding diagram of diborane (B_2H_6) showing with curved lines a pair of 3-center 2-electron bonds.



William N. Lipscomb

Lipscombite

Carboxypeptidase A



Aspartate carbamoyl transferase

The Nobel Prize in Chemistry 1976 was awarded to William Lipscomb *"for his studies on the structure of boranes illuminating problems of chemical bonding".*

The Nobel Prize in Chemistry 1985

Herbert A. Hauptman, Jerome Karle

The Nobel Prize in Chemistry 1985

Herbert A. Hauptman

Jerome Karle

$$F_{hkl} = \sum_{h'k'l'} F_{h'k'l'} F_{h-h',k-k',l-l'}$$

Sayre equation

$$S_h \approx S_{h'} S_{h-h'}$$

Direct methods are the preferred method for phasing crystals of small molecules having up to 1000 atoms in the asymmetric unit. Hauptman and Karle developed a practical method to employ the Sayre equation to exploit statistical correlations between the phases of different Fourier components that result from the fact that the scattering density must be a positive real number.

The Nobel Prize in Chemistry 1985 was awarded jointly to Herbert A. Hauptman and Jerome Karle *"for their outstanding achievements in the development of direct methods for the determination of crystal structures"*

The Nobel Prize in Chemistry 1988

Johann Deisenhofer, Robert Huber, Hartmut Michel

The Nobel Prize in Chemistry 1988

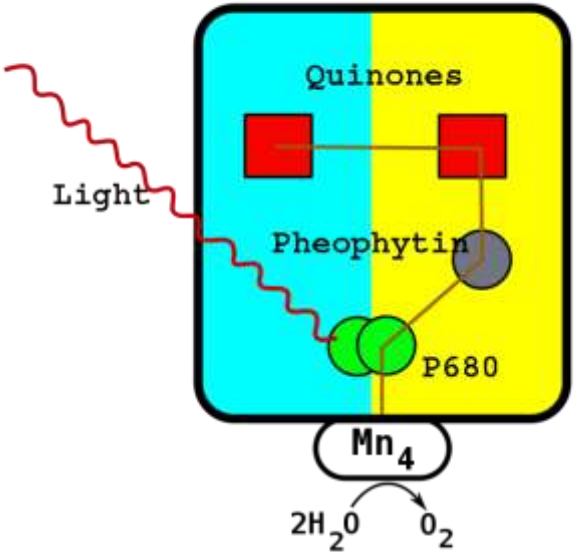
Johann Deisenhofer

Robert Huber

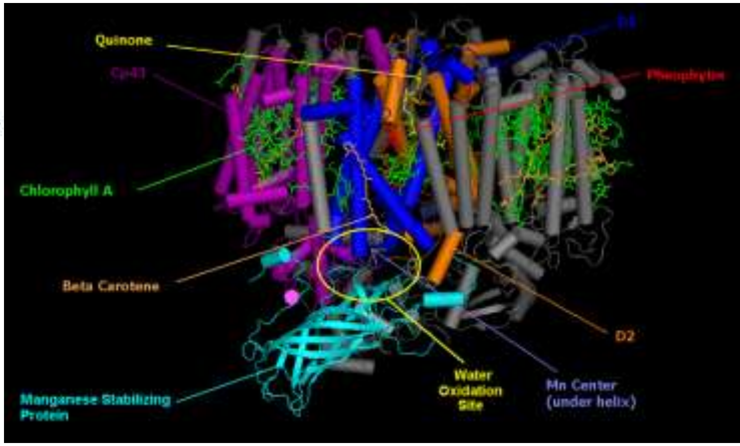
Hartmut Michel

The Nobel Prize in Chemistry 1988 was awarded jointly to Johann Deisenhofer, Robert Huber and Hartmut Michel *"for the determination of the three-dimensional structure of a photosynthetic reaction centre"*.

$$2Q + 2H_2O \overset{light}{\Longrightarrow} O_2 + 2QH_2$$

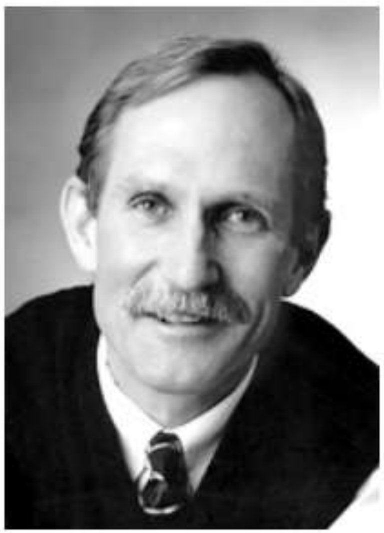


Photoreaction Center



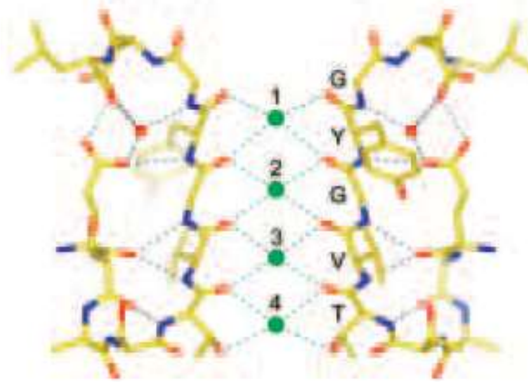
The Nobel Prize in Chemistry 2003
Peter Agre, Roderick MacKinnon

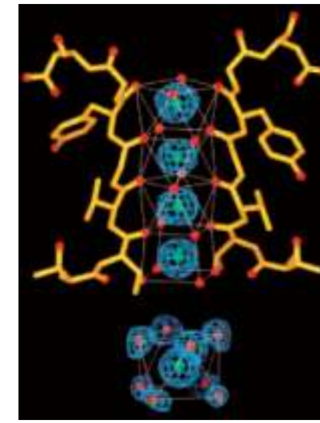
The Nobel Prize in Chemistry 2003



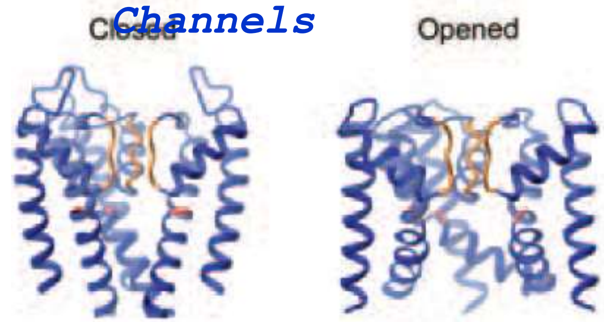
Peter Agre

Roderick MacKinnon





Potassium Ion Channels



The Nobel Prize in Chemistry 2003 was awarded *"for discoveries concerning channels in cell membranes"* jointly with one half to Peter Agre *"for the discovery of water channels"* and with one half to Roderick MacKinnon *"for structural and mechanistic studies of ion channels"*.

The Nobel Prize in Chemistry 2009
Venkatraman Ramakrishnan, Thomas A. Steitz, Ada E. Yonath

international year of crystallography 2014

The Nobel Prize in Chemistry 2009

Photo: U. Montan

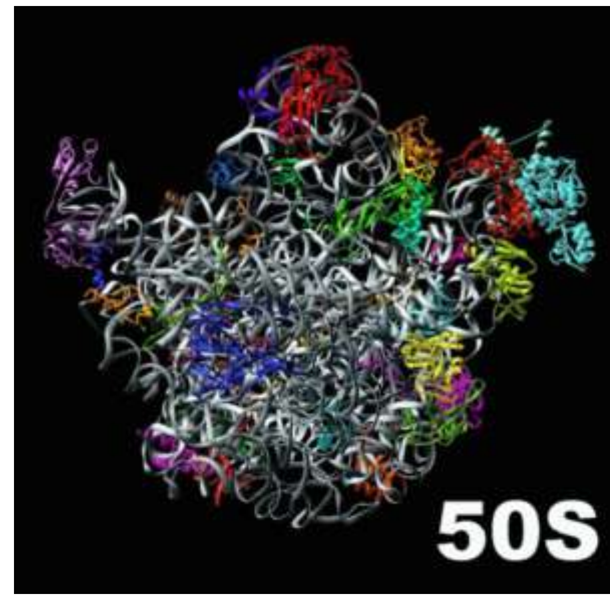
Venkatraman Ramakrishnan

Photo: U. Montan

Thomas A. Steitz

Photo: U. Montan

Ada E. Yonath



Ribosome

The Nobel Prize in Chemistry 2009 was awarded jointly to Venkatraman Ramakrishnan, Thomas A. Steitz and Ada E. Yonath *"for studies of the structure and function of the ribosome"*.

The Nobel Prize in Chemistry 2011
Dan Shechtman

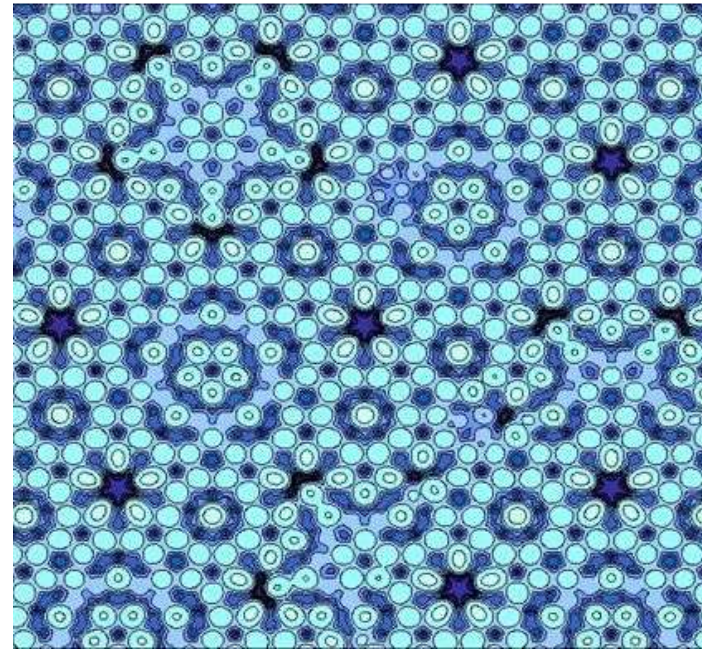
2014 international year of crystallography IUCr

The Nobel Prize in Chemistry 2011

Dan Shechtman

Linus Pauling –
"There is no such thing as quasicrystals, only quasi-scientists."

Quasicrystals have low thermal and electrical conductivity, while possessing high structural stability – ideal for non-stick insulation for electrical wires and cooking equipment.



Quasicrystals – ordered crystalline materials lacking repeating structures, such as this Al-Pd-Mn alloy.

The Nobel Prize in Chemistry 2011 was awarded to Dan Shechtman *"for the discovery of quasicrystals"*.

The Nobel Prize in Chemistry 2013
Martin Karplus, Michael Levitt, Arieh Warshel

The Nobel Prize in Chemistry 2013

© Harvard University
Martin Karplus

Photo: © S. Fisch
Michael Levitt

Photo: Wikimedia Commons
Arieh Warshel

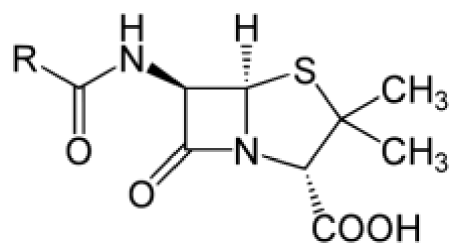
The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel *"for the development of multiscale models for complex chemical systems"*.

The Nobel Prize in Chemistry 1964

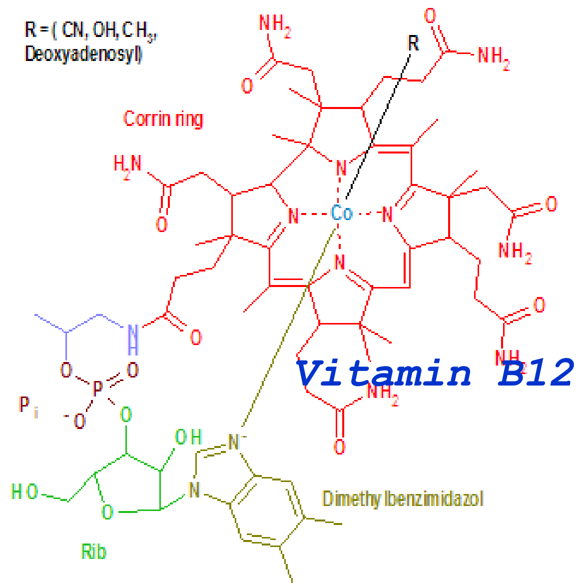
Dorothy Crowfoot Hodgkin

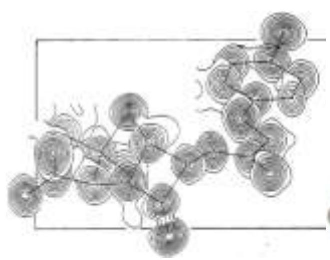
The Nobel Prize in Chemistry 1964

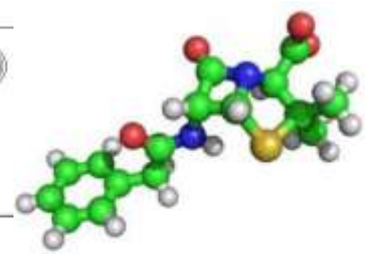
Dorothy Crowfoot Hodgkin

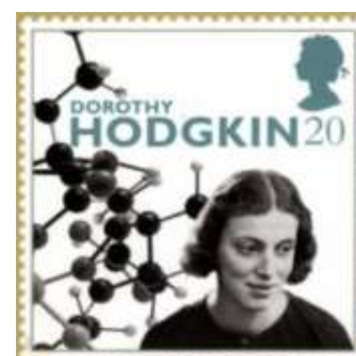


Penicillin



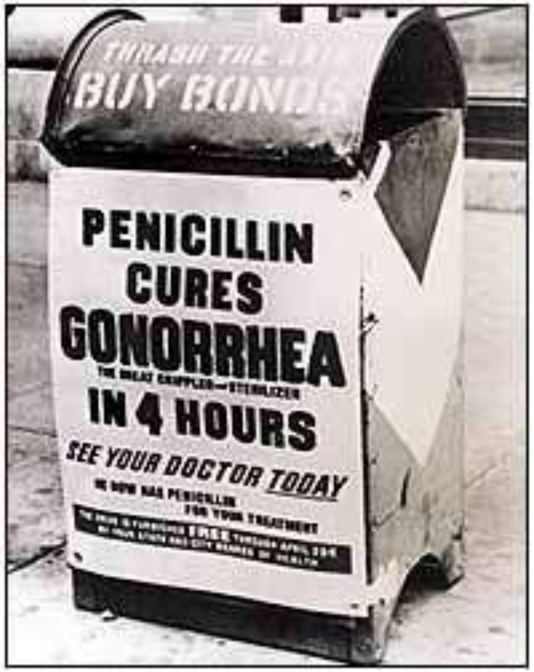






The Nobel Prize in Chemistry 1964 was awarded to Dorothy Crowfoot Hodgkin *"for her determinations by X-ray techniques of the structures of important biochemical substances"*.

The Good Old Days…



modern headlines:

The ticking time bomb…
The serious threat…
escalating antibiotic resistance…
untreatable bacterial infections…

Doug Mitchell, Univ. of Illinois at Urbana-Champaign

- Alexander Fleming (Scottish scientist) fought in World War I. His battlefront experience showed him how dangerous bacteria could be to human life. After the war he spent most of his time at **St. Mary's Hospital in London** doing research, focusing on finding a chemical that would stop bacterial infection.

- He discovered lysozyme, an enzyme occurring in many body fluids, such as tears. It had a natural antibacterial effect, but not against the strongest infectious agents (*e.g.* ***Staphylococcus aureus***). Fleming's research focused on finding agents that would kill this particular bacterium.

- In the Fall of 1928, Fleming had prepared ***Staphylococcus*** on several plates and forgot to put them in the incubator before he went on vacation.

- When he returned from vacation, he discovered that one of the plates was contaminated with molds. This was not unusual; it had happened all the time. He knew that this contamination must have come from the floor below, because at that time there was a group there working with molds. **But what was unusual about this particular strain of molds was that it killed the *Staphylococcus* in the surrounding area.**

- It turned out that the reasons why Fleming was able to observed this effect were: (1) this particular mold strain (later identified to be *Penicillium notatum*) was a **good producer of penicillin**, and (2) the **temperature was unusually cold at that time of year**, which caused the mold and bacteria to grow very slowly (necessary to observe the inhibiting effect).

- For the next 7 years, Fleming and his colleagues tried to produce large quantities of penicillin so that it could be tested in animals and humans, but they not very successful.

- In 1935, **Howard Florey** was appointed professor of pathology at **Oxford** and he hired **Ernst Chain** to work on a cancer-related project. Chain had read the article previously published by Fleming and tried to convince Florey to revisit the penicillin problem (Fleming claimed that it was unstable and that was the reason he could not get enough to do animal or human trials).

- The Florey team began working on penicillin in full force. **Every bucket, container, bottle they could find were used** to culture *Penicillium notatum*. By **May 1940, the team produced enough penicillin to test on infected animals for the first time**. Eight mice were infected with a lethal dose of *Staphylococcus*. One hour later, four of them were injected with penicillin and the other four were left without treatment. All four mice that did not receive penicillin died in less than 24 h. All four mice treated with penicillin were health. Florey proclaimed, "**it looks like a miracle**".

- **To do test on humans, the amount of pencillin required was 3,000 times greater**. By now, **England was at war** and financial resources were limited. A creative solution would have to be developed in order to produce penicillin in large quantity. **Heatly, a team member, designed a container that resembles a bedpan out of ceramic, suited for their need**. **400 stackable containers were made and this allowed them to produce enough penicillin to do test on human for the first time**. Although the first patient treated with penicillin died due to a shortage of supply, further tests showed that penicillin successfully treats human infections as well.

- Florey tried to get British pharmaceutical companies to produce penicillin, but failed (mainly because the war had greater demand for other supplies).

- **In 1941, Florey and Heatly** came to the US to convince American pharmaceutical companies to produce penicillin. **They ended up in Peoria, Illinois**. **An agriculture research center there had developed excellent techniques of fermentation** (a process needed for penicillin growth). The nutrients used for penicillin growth there was **corn**, which was not commonly grown in Britain. **The penicillin-producing mold loved corn and produced 500 times as much as it had produced before**.

- **The first batches of this new wonder drug** became available in **1943** and were reserved for military use. News of penicillin was suppressed because of the war.

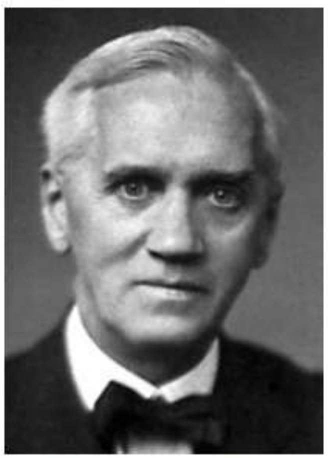
- When it was first released, **it was so valuable that patients' urine was collected and the excreted penicillin purified to be used again**.

- By this time, the US had entered World War II. **The government recruited 21 chemical companies to produce penicillin**. **From January to May 1943, only 400 million units of penicillin were made; by the time the war ended, US companies were making 650 <u>billion</u> units a month.**

- Penicillin kills bacteria by interfering with aminopetidase, an enzyme responsible for making bacteria cell wall. Human and mammals do not have this enzyme.

The Nobel Prize in Physiology or Medicine 1945
Sir Alexander Fleming, Ernst B. Chain, Sir Howard Florey

The Nobel Prize in Physiology or Medicine 1945



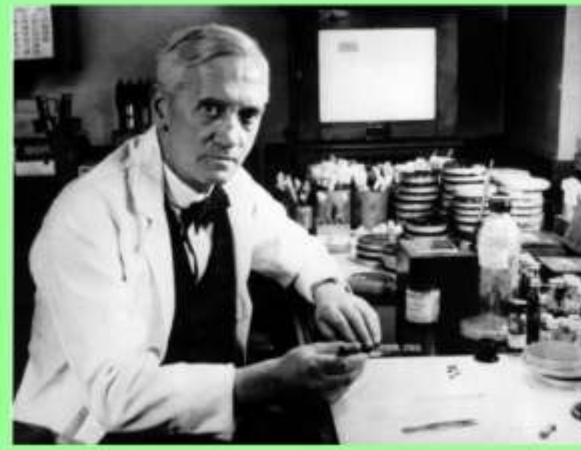
Sir Alexander Fleming

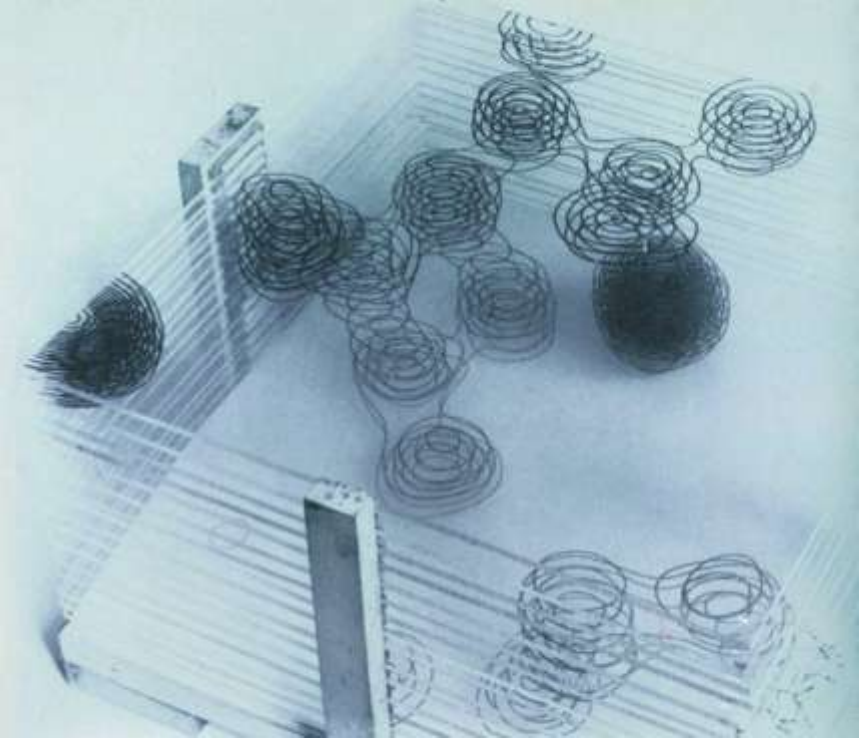
Ernst Boris Chain

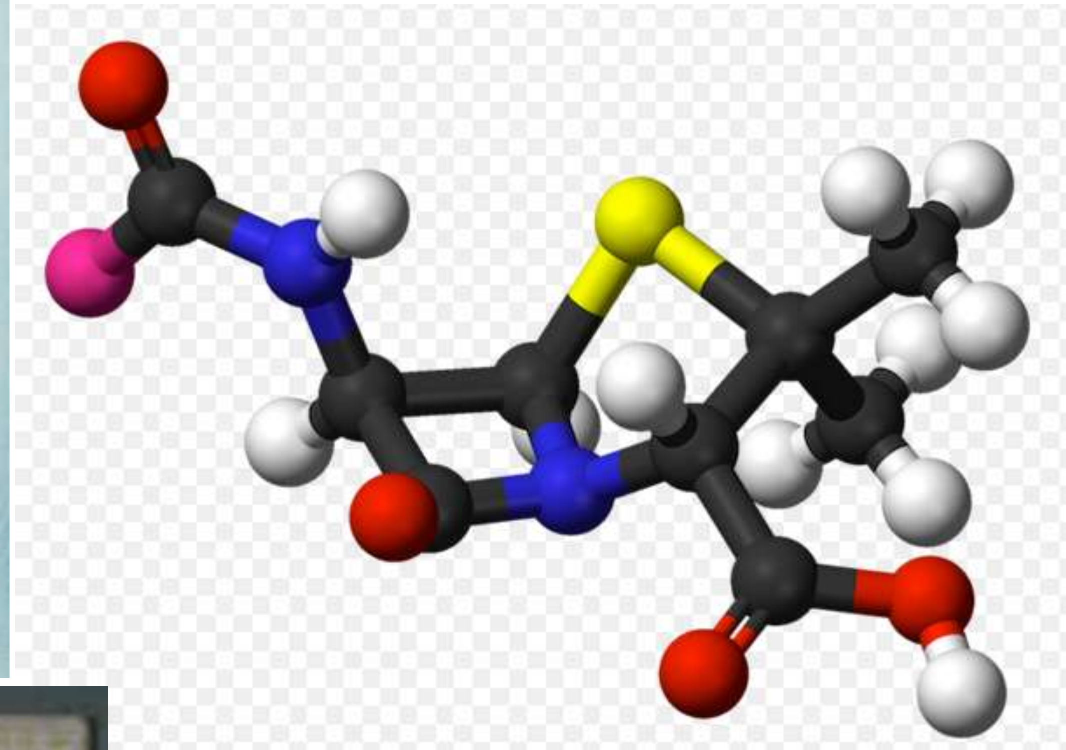
Sir Howard Walter Florey

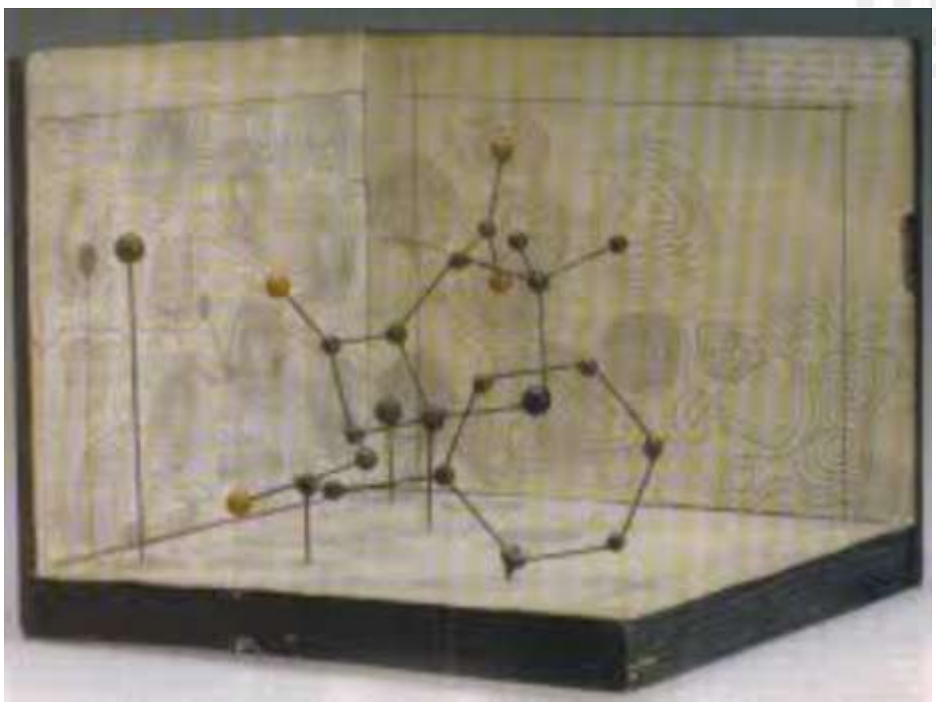
The Nobel Prize in Physiology or Medicine 1945 was awarded jointly to Sir Alexander Fleming, Ernst Boris Chain and Sir Howard Walter Florey *"for the discovery of penicillin and its curative effect in various infectious diseases"*.

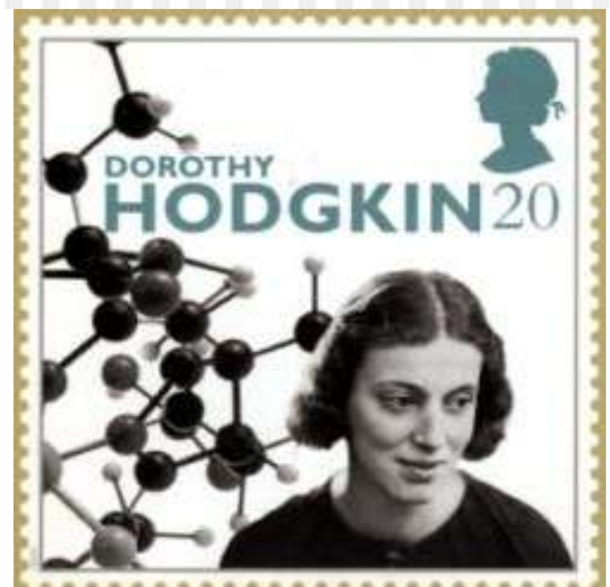
Alexander Fleming and Penicillin: The Accidental Discovery?










DOROTHY
HODGKIN 20

Diamond

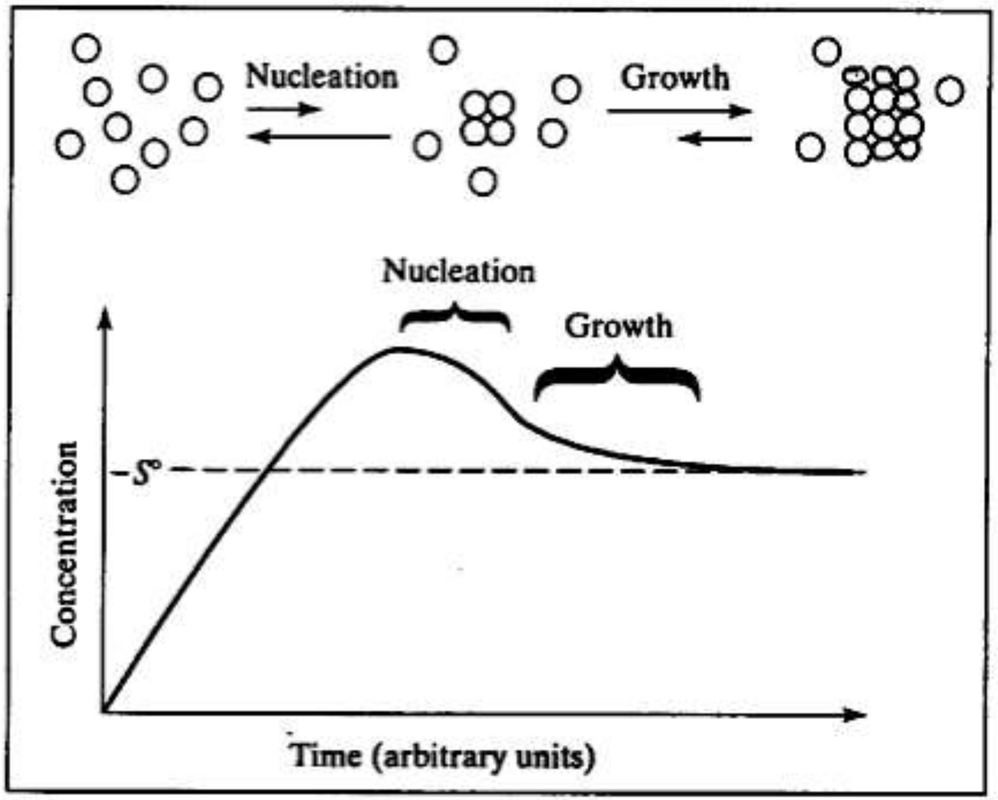
Pink Diamond

Uncut Diamond

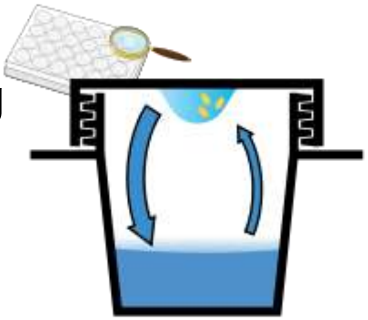
Crystals

Growing protein crystals.

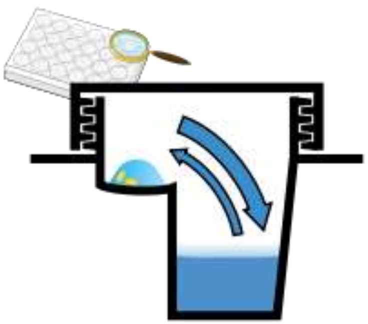
Methods to slowly change solution conditions



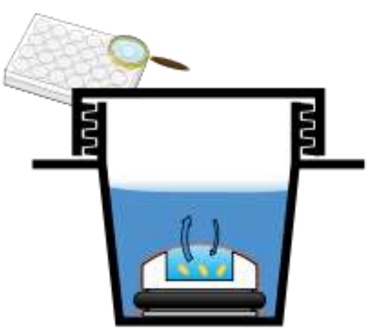
Hanging Drop



Sitting Drop



Micro-dialysis



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

Common Compounds used in Crystallization

Ammonium sulfate / or sodium

Sodium or ammonium citrate
Sodium or ammonium acetate
Magnesium sulfate
Cetyltrimethyl ammonium salts

Polyethylene glycol 400, 1000, 2000, 4000, 6000, 8000, 15,000 M

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

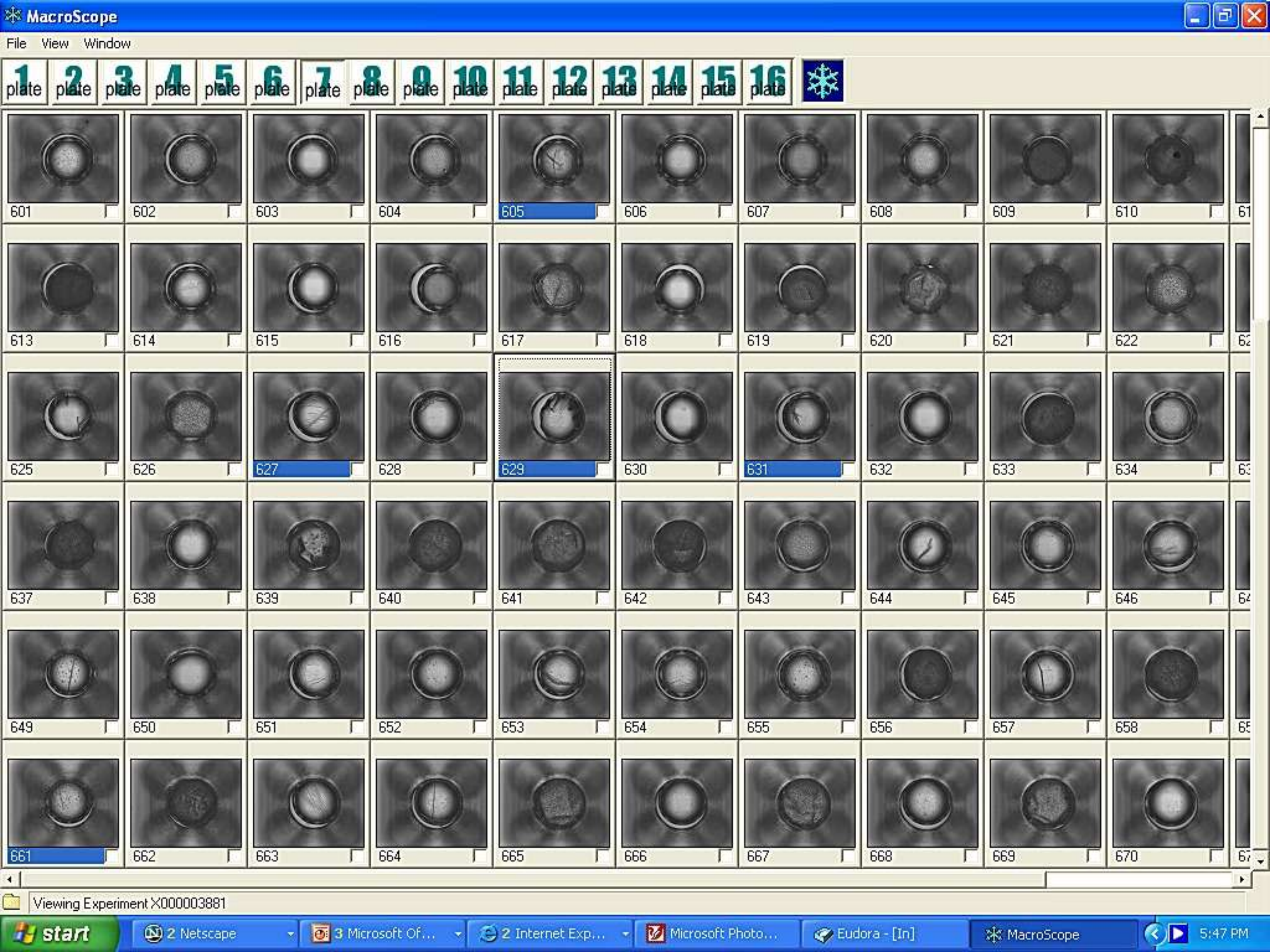
Hanging Drop Method - Crystal Screening

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.

Hampton Crystal Screen Solutions

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


MacroScope
File View Window
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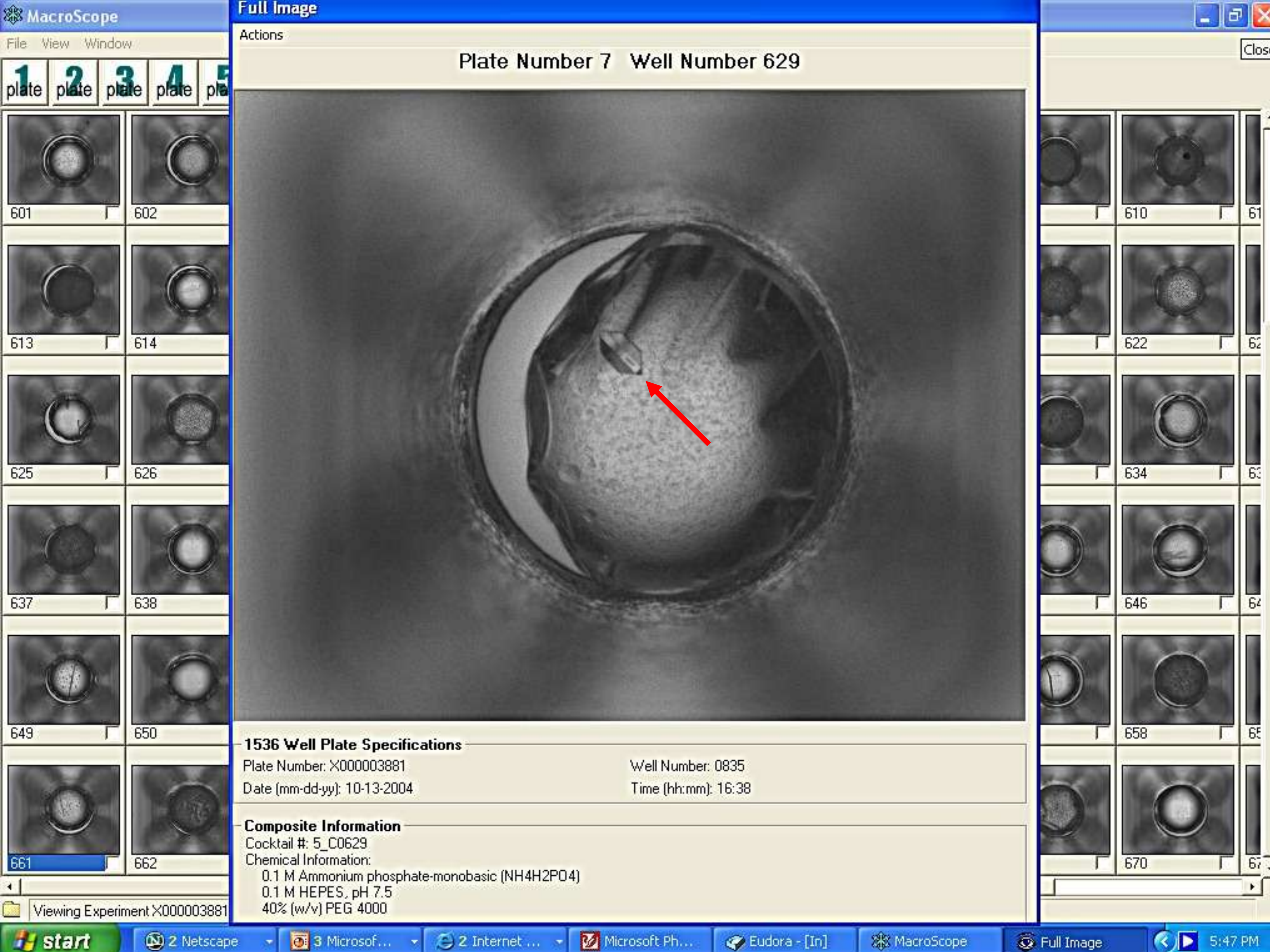
MacroScope
File View Window
Full Image
Actions
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1536 Well Plate Specifications
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Well Number: 0835
Date (mm-dd-yy): 10-13-2004
Time (hh:mm): 16:38
Composite Information
Cocktail #: 5_C0629
Chemical Information:
0.1 M Ammonium phosphate-monobasic (NH4H2PO4)
0.1 M HEPES, pH 7.5
40% (w/v) PEG 4000
Viewing Experiment X000003881
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3 Microsof...
2 Internet ...
Microsoft Ph...
Eudora - [In]
MacroScope
Full Image
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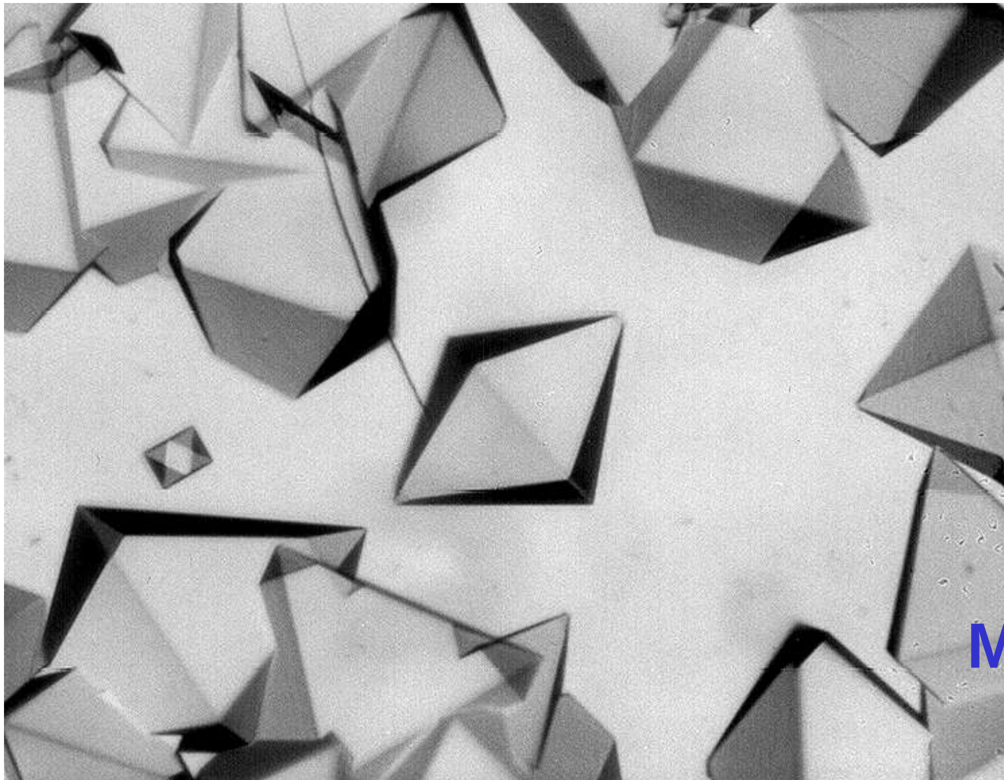
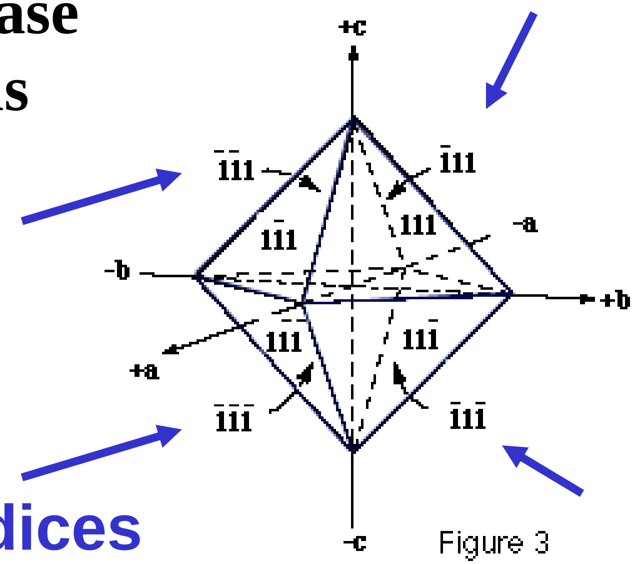
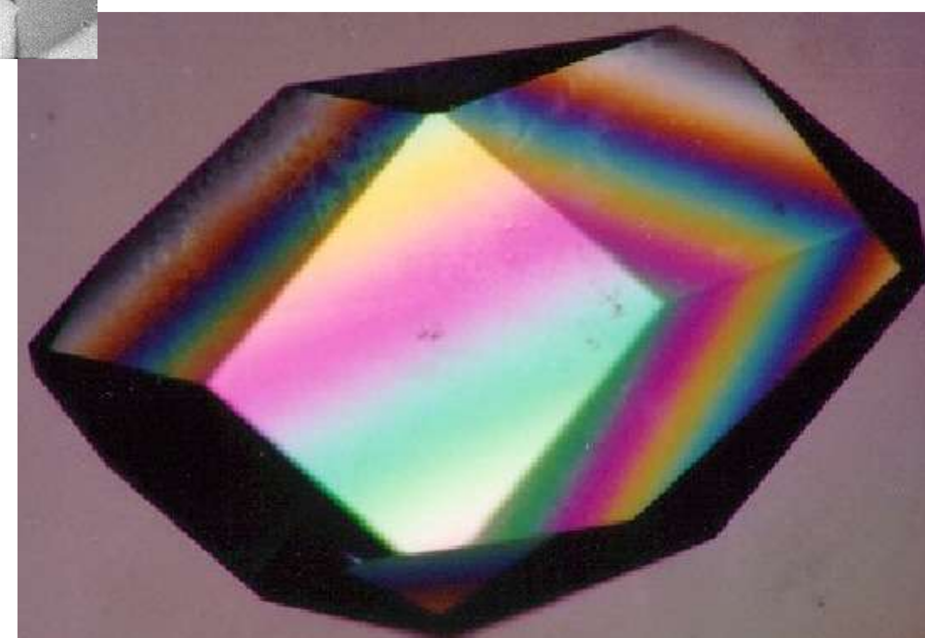


Glucose Isomerase Crystals



Miller Indices



Lysozyme Crystals

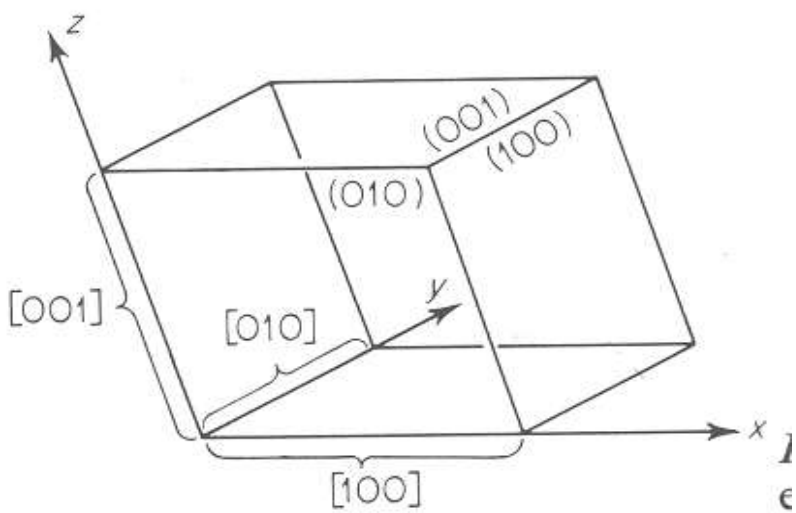
Bragg Planes

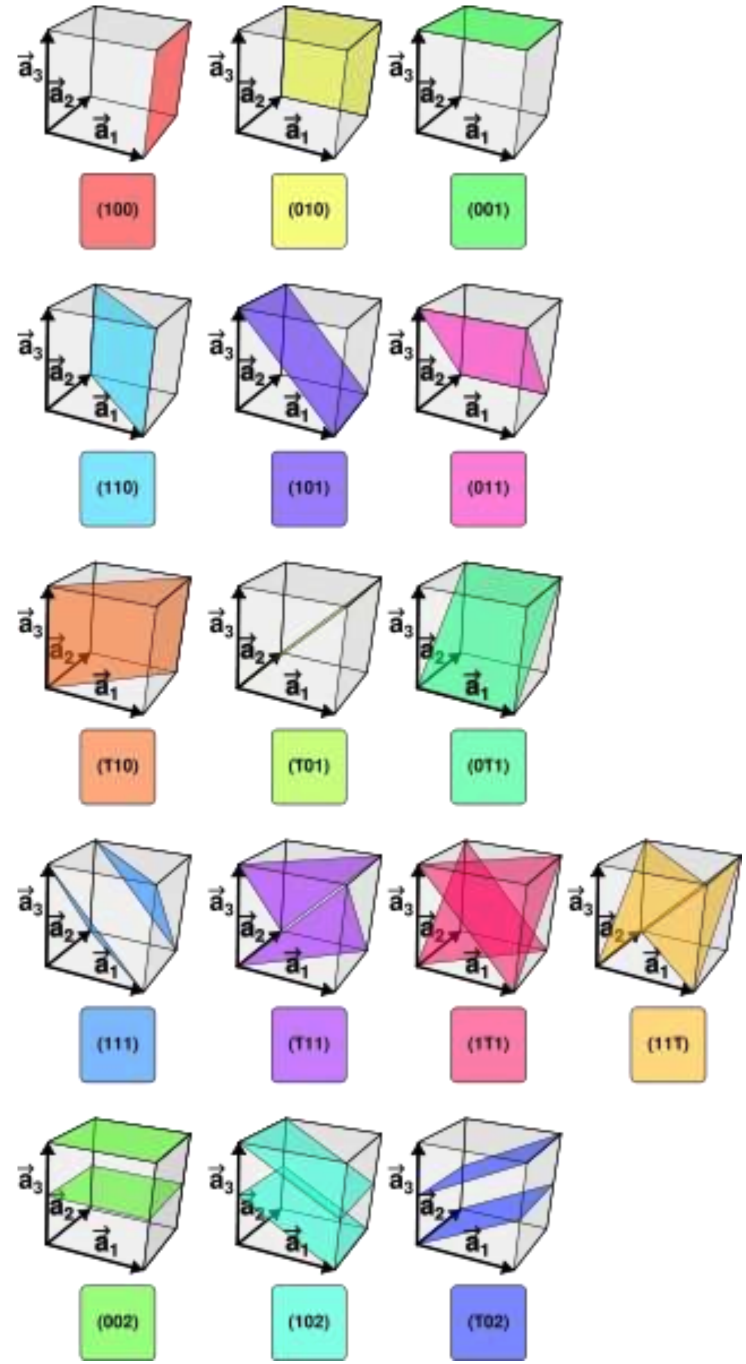
X-ray scattering can be understood as if the x-rays are reflected from planes in the crystal.

h, k, l are integers, called “Miller indices”

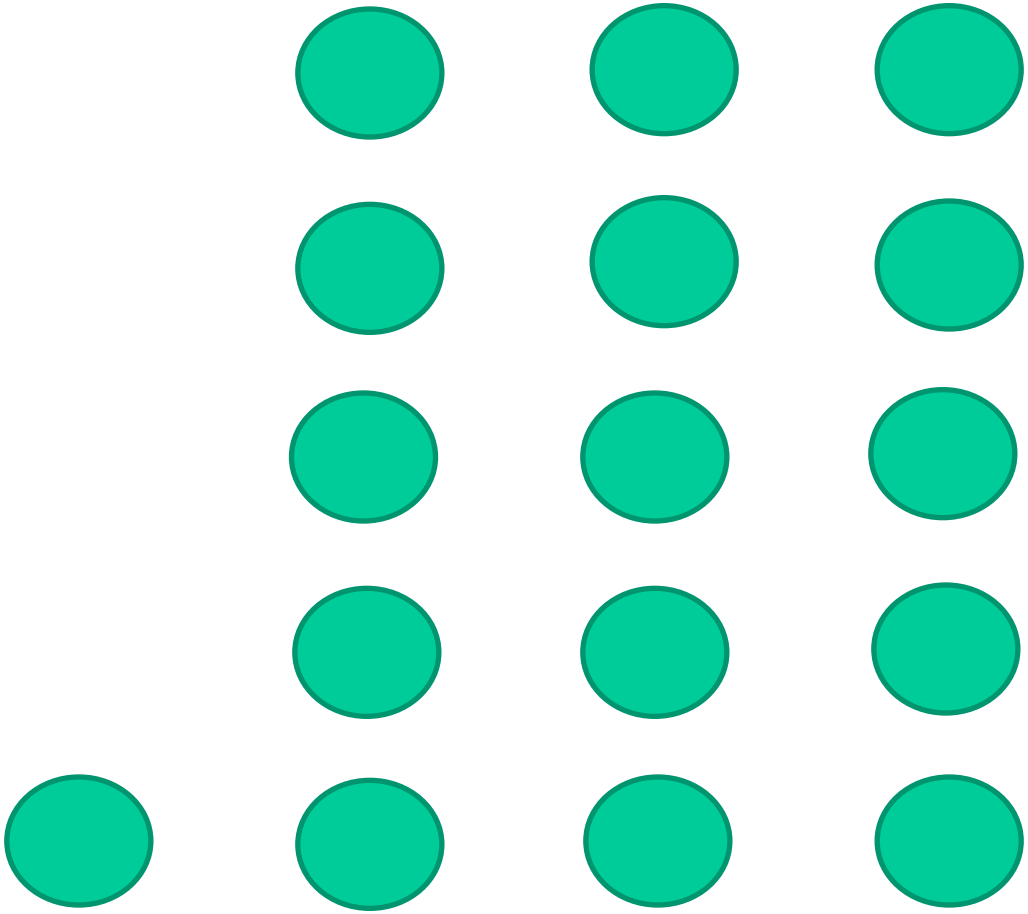
Miller indices are used to define the direction of planes within a crystal. A plane with Miller indices h,k,l intersects the unit cell edges a,b,c at points a/h, b/k and c/l.

(3 integers define the direction of a plane).

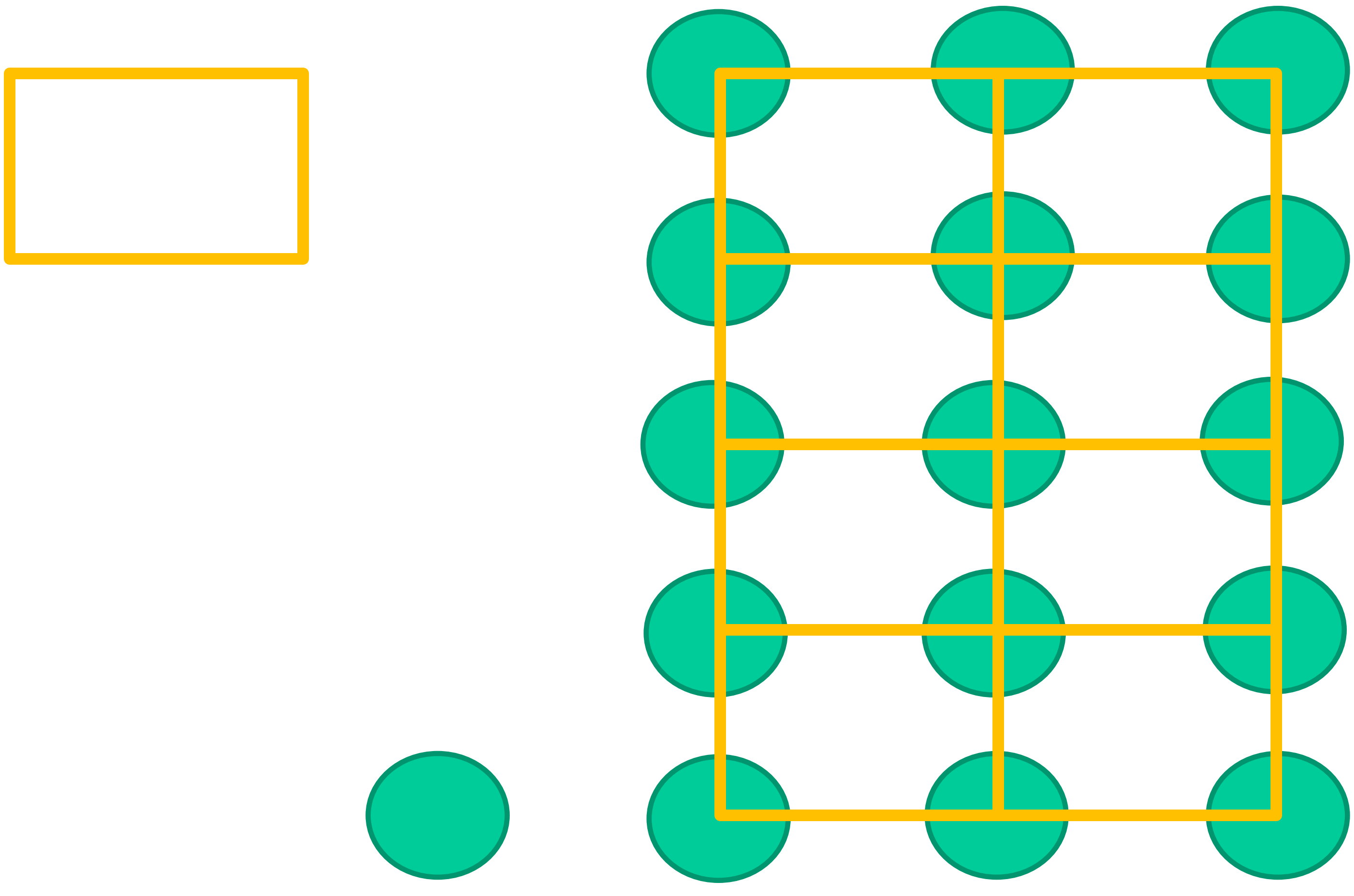




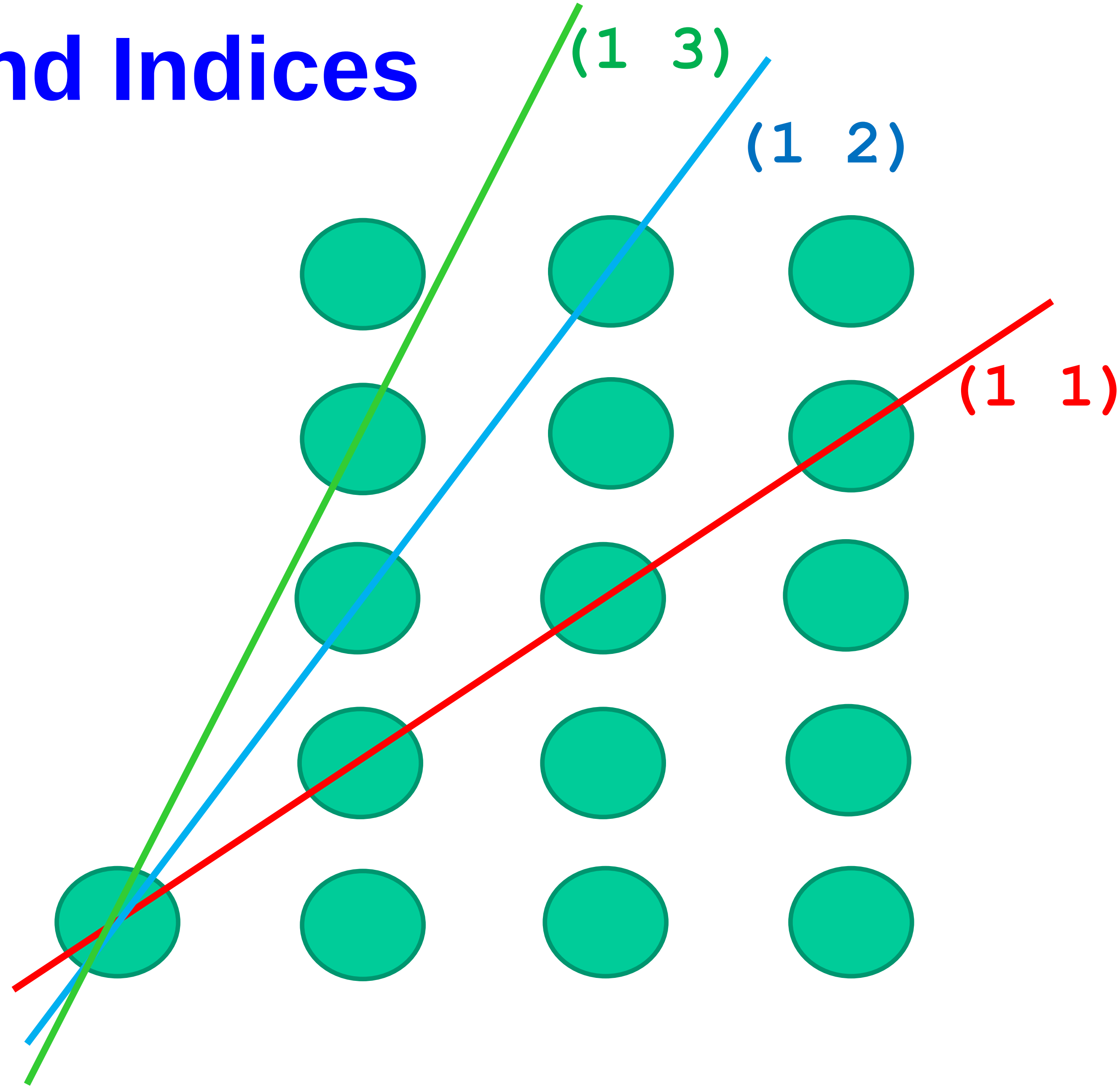
Atoms in space



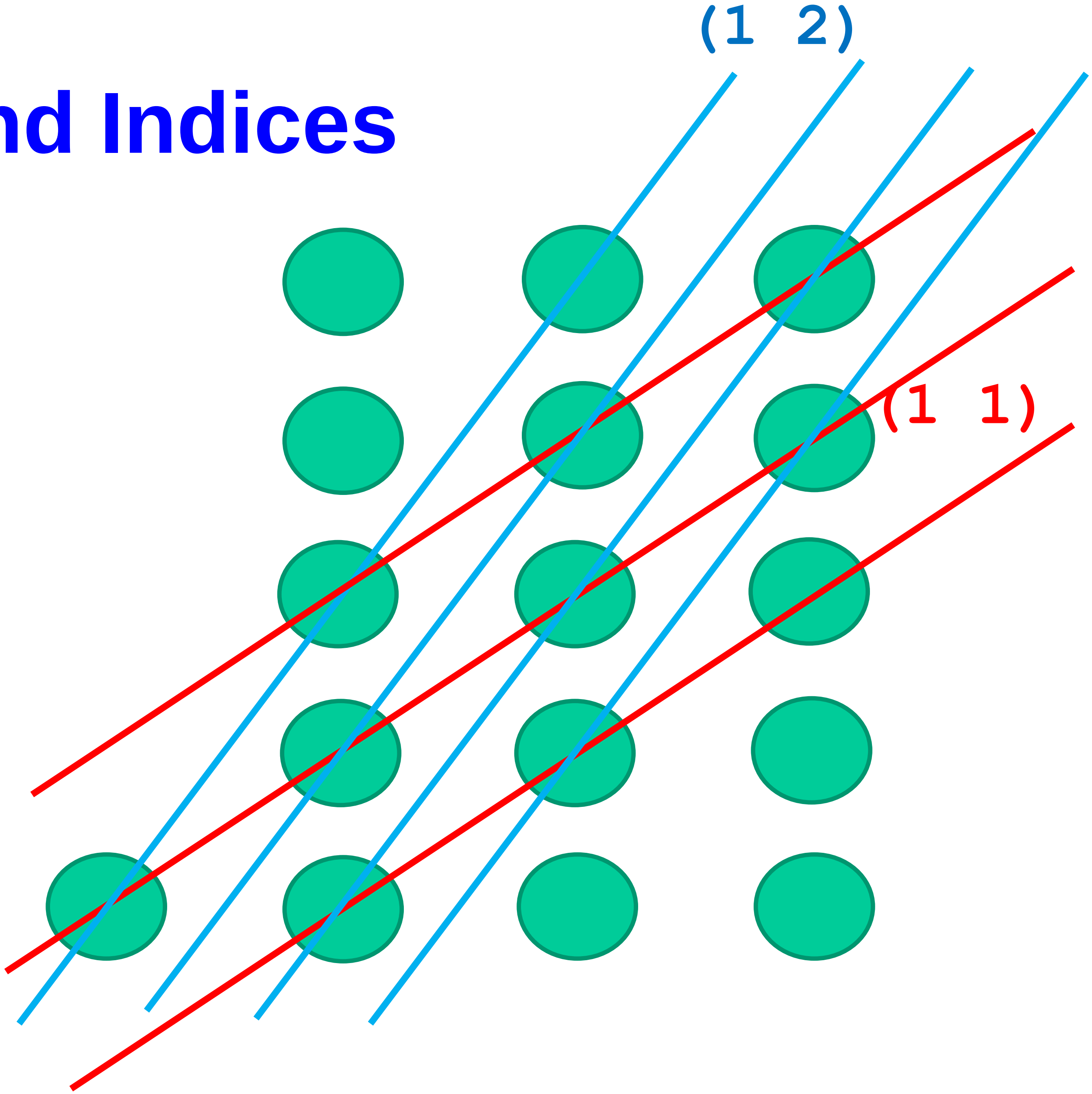
Atoms in space / Unit Cell



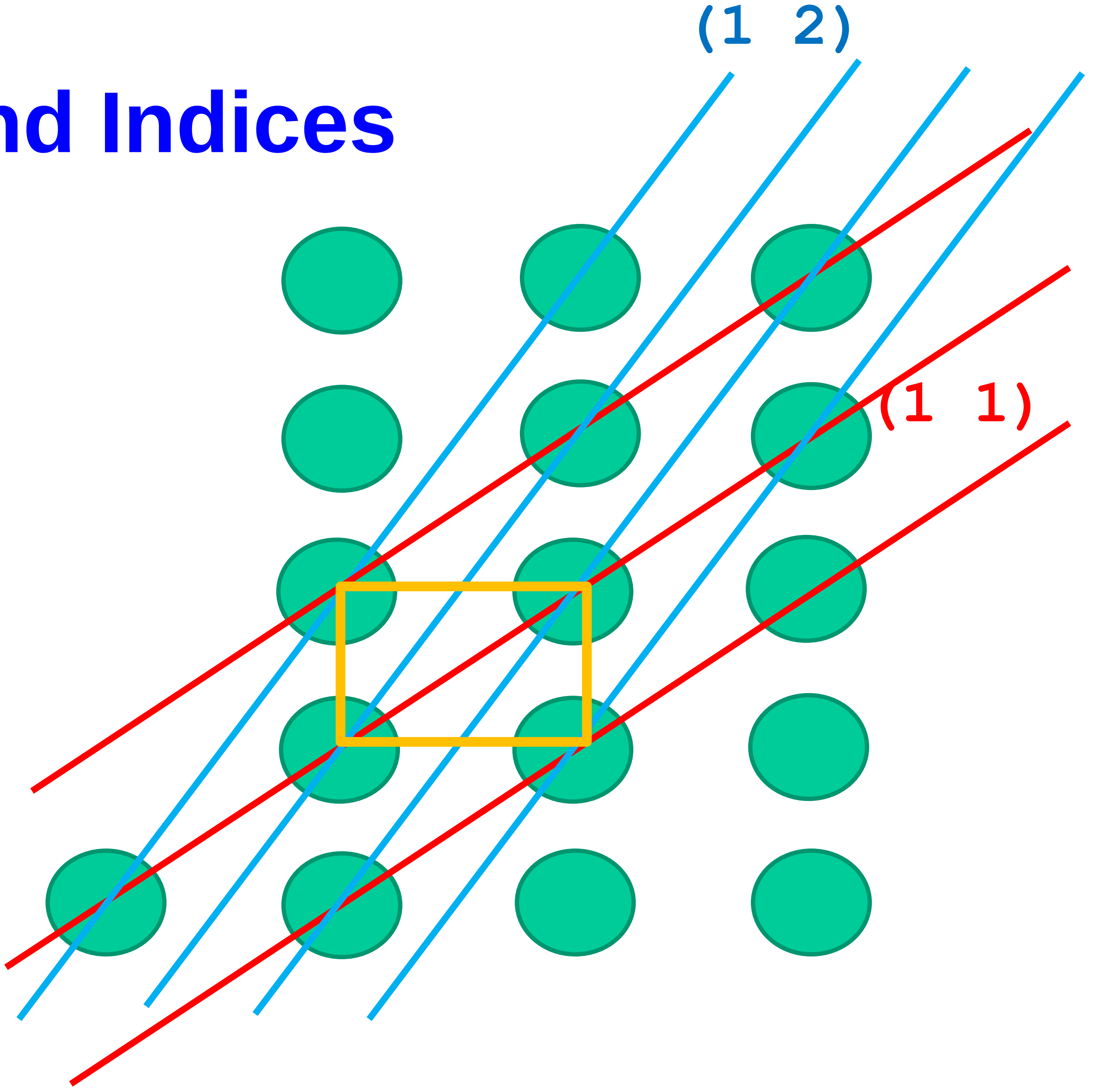
Planes and Indices



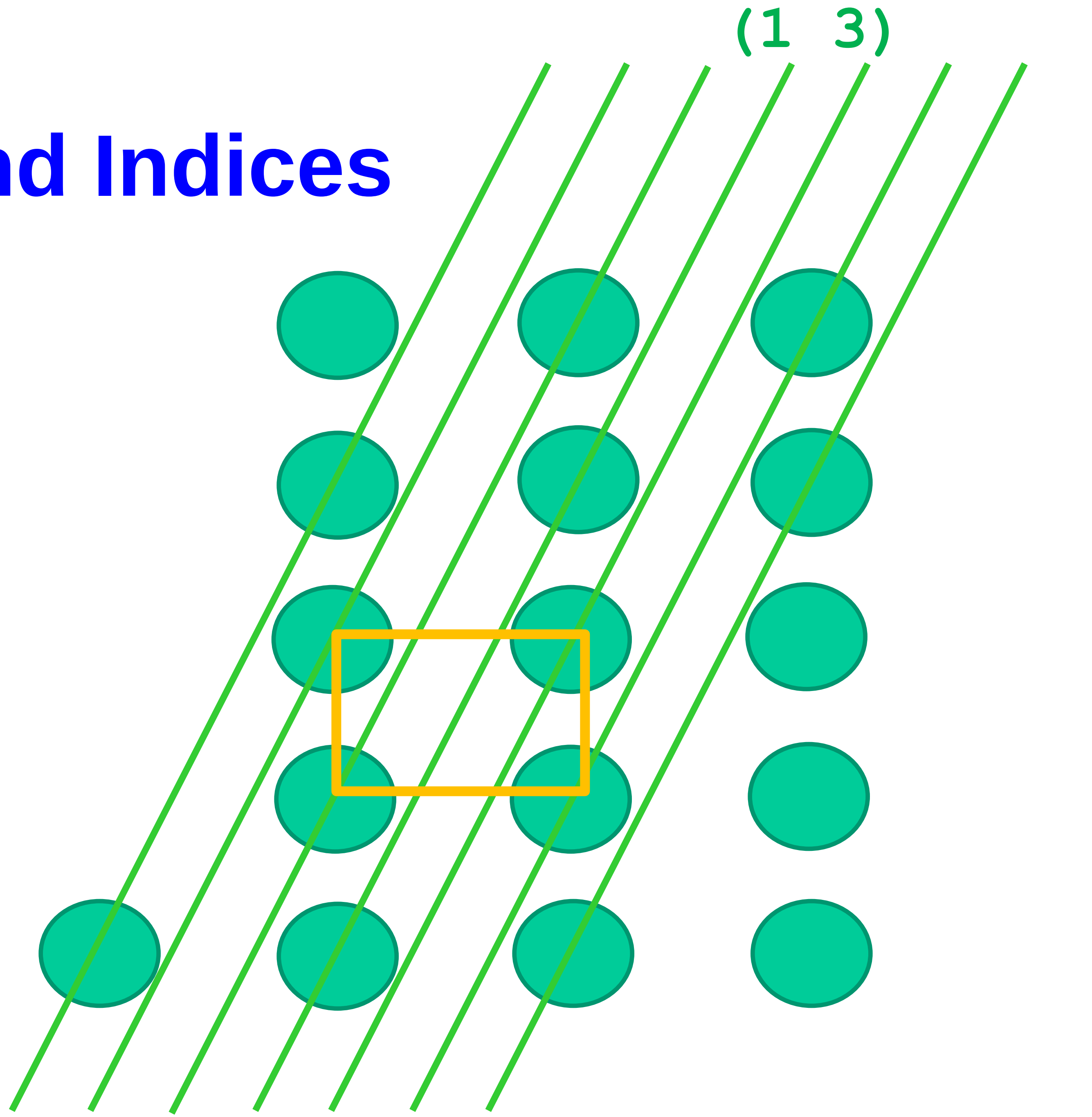
Planes and Indices



Planes and Indices



Planes and Indices



Name that Bragg "plane"

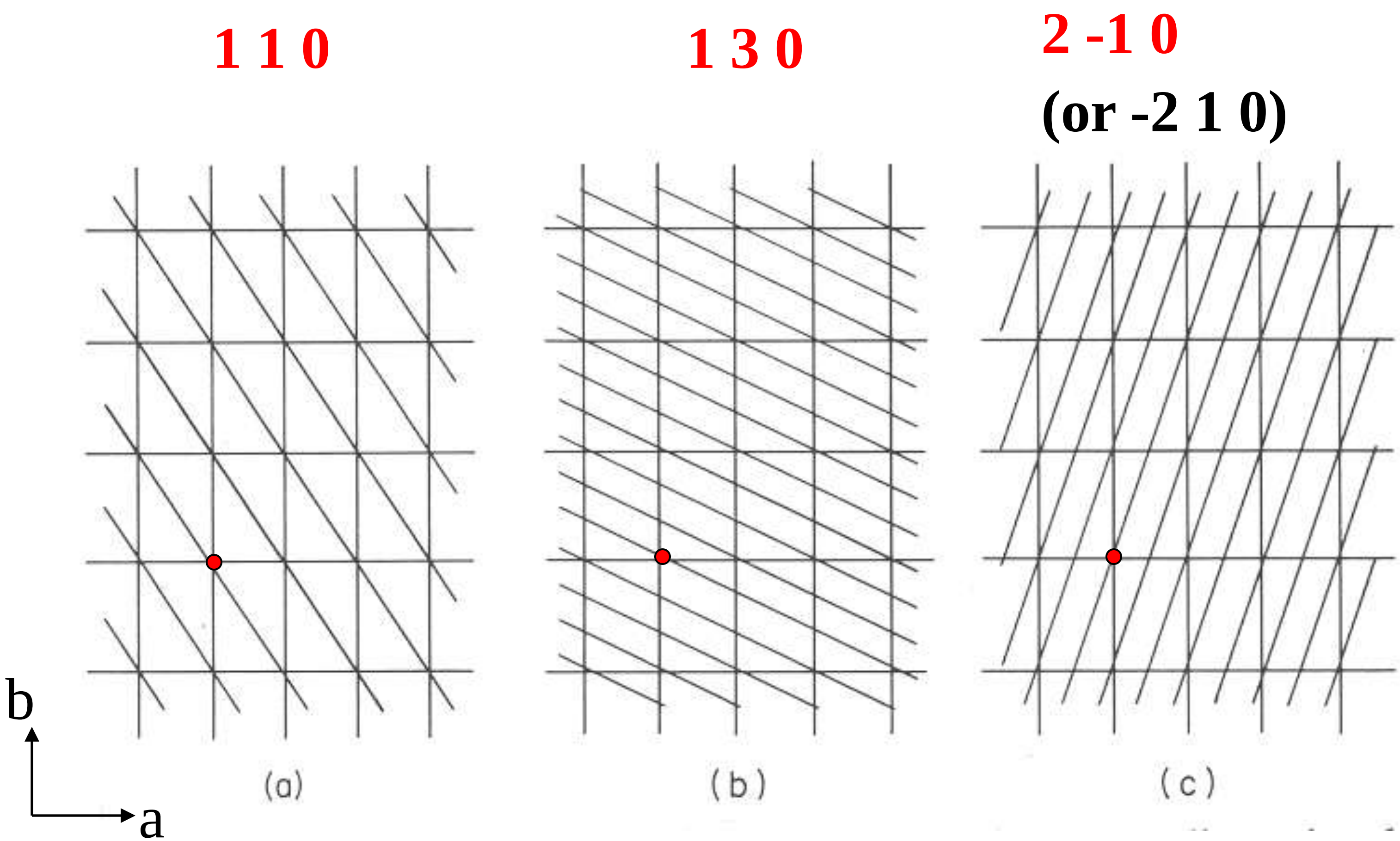
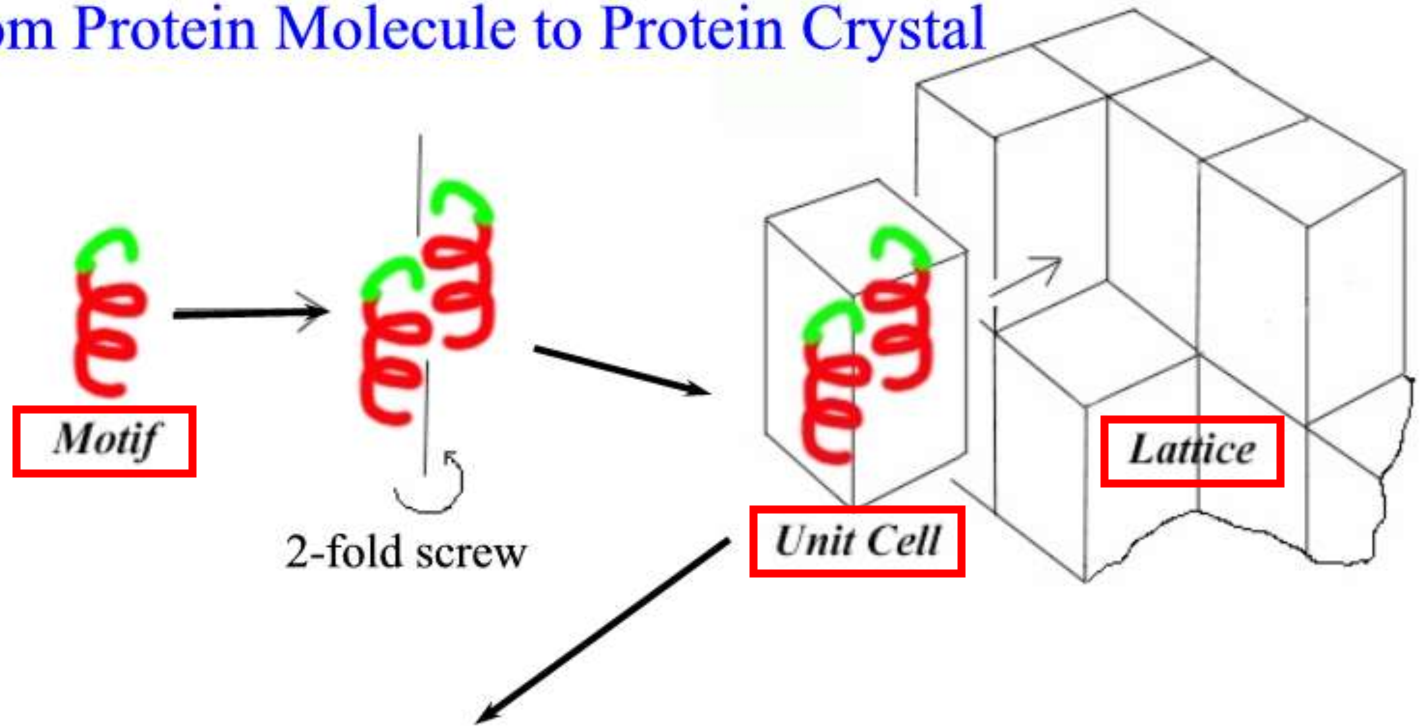
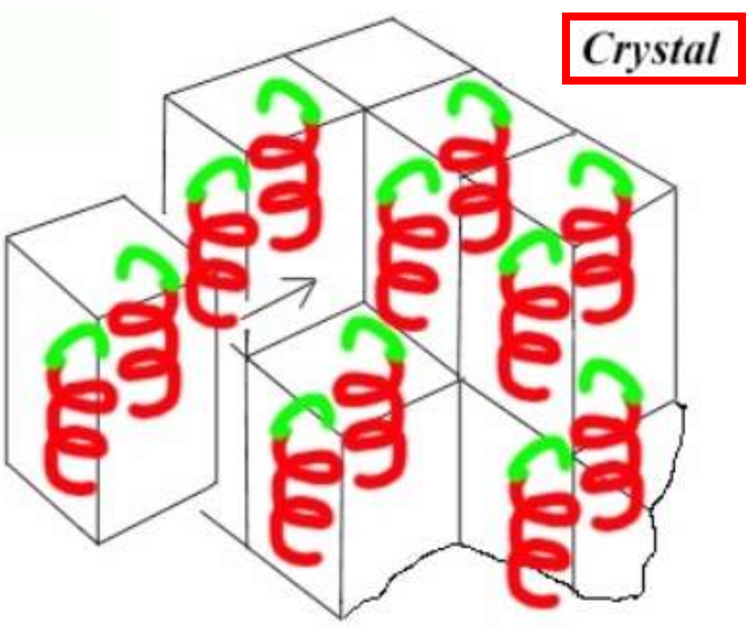
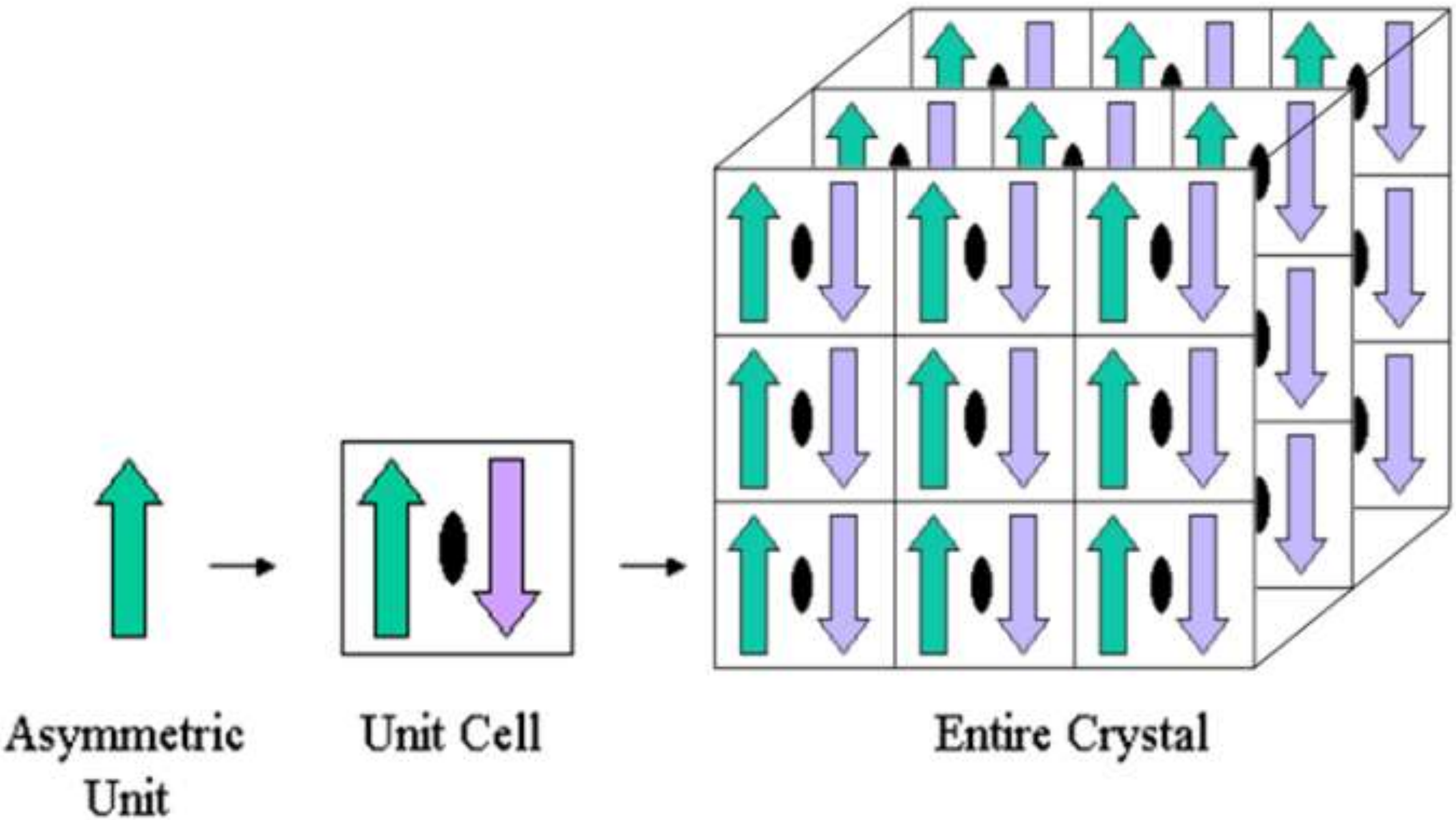


Figure 2.5. Three families of lattice "planes" in a two-dimensional lattice.

From Protein Molecule to Protein Crystal






Asymmetric
Unit
Unit Cell
Entire Crystal

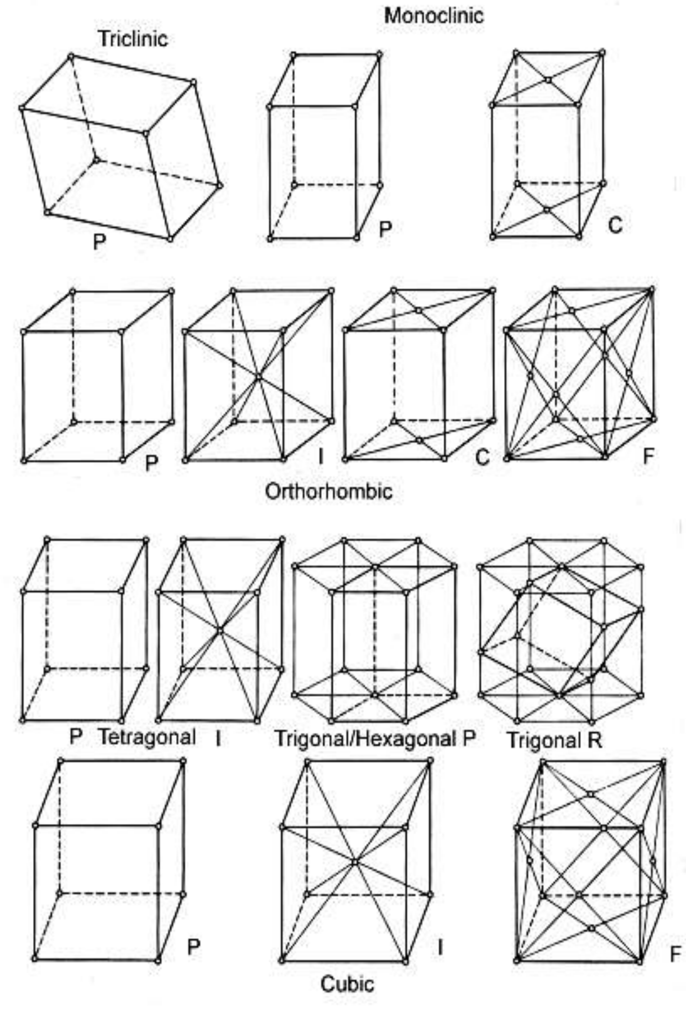
Crystal Systems

Crystal System	Bravais Type(s)	External Minimum Symmetry	Unit Cell Properties
Triclinc	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
Triclinc	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, Pm-3m, Fm-3m, Im-3m

The 14 Bravais Lattices



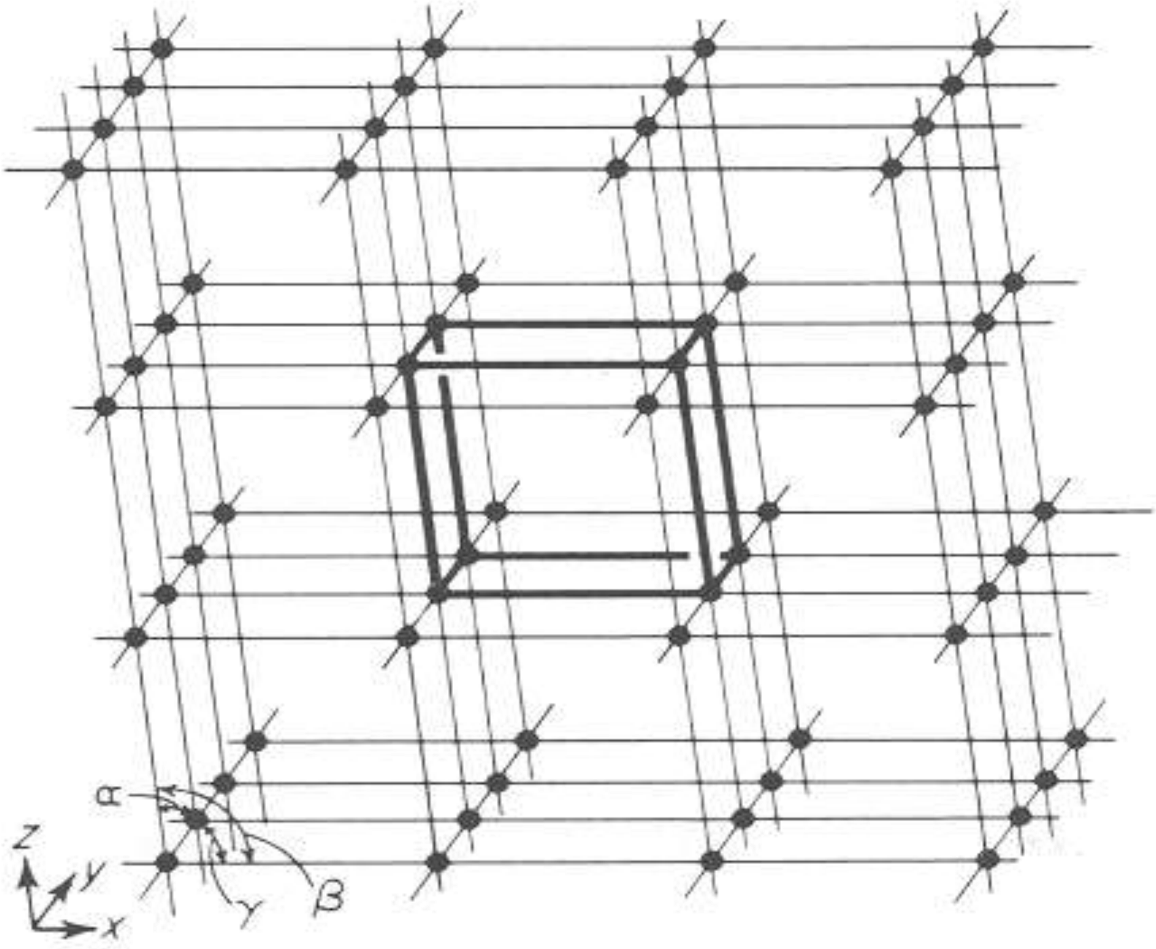
Notes

Note: Only 2-, 3-, 4-, and 6-fold rotations allowed

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

A unit cell is defined by its lattice constants:

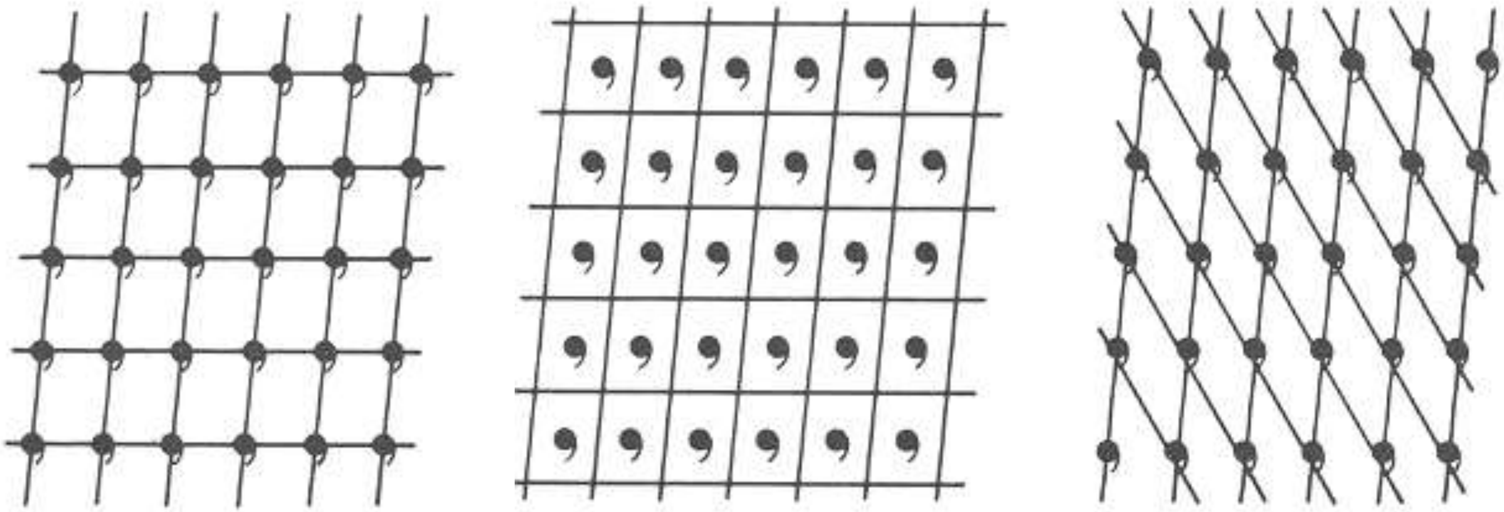
a, b, c and α, β, γ



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

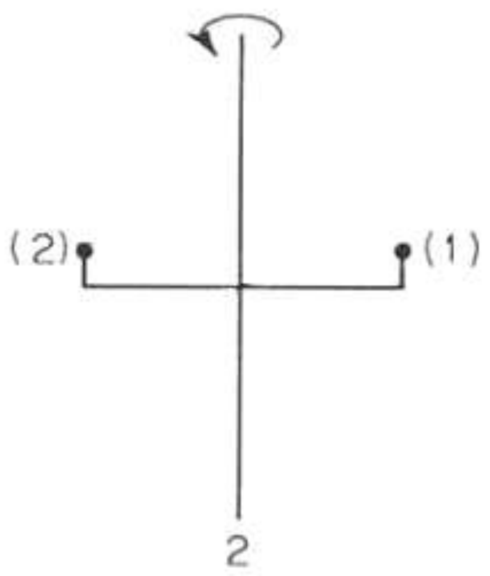
How to identify “the” unit cell ?

Regular two-dimensional array.

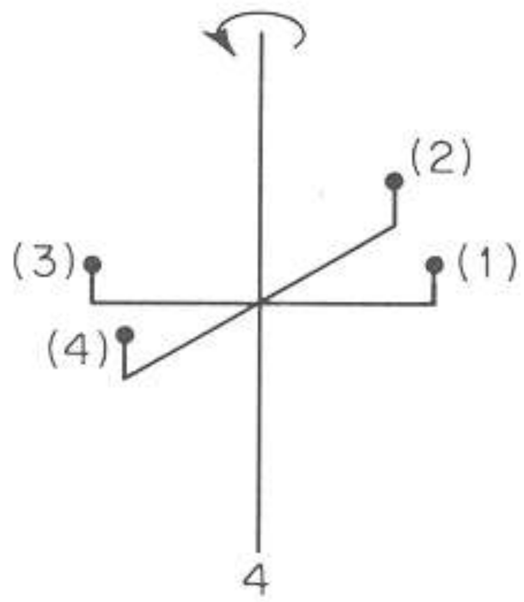


Three different grid systems referred to the array same array.

How to identify "the" unit cell ? Role of Symmetry



A 2-fold rotation axis.



A 4-fold rotation axis.

Rotation axes:	**2-fold**	**3-fold**	**4-fold**	**6-fold**
	180°	120°	90°	60°
Translations:	1/2	1/3	1/4	1/6

Rot + Trans (Screw Axes) / Mirror / Inversion

How to identify "the" unit cell ? Role of Symmetry

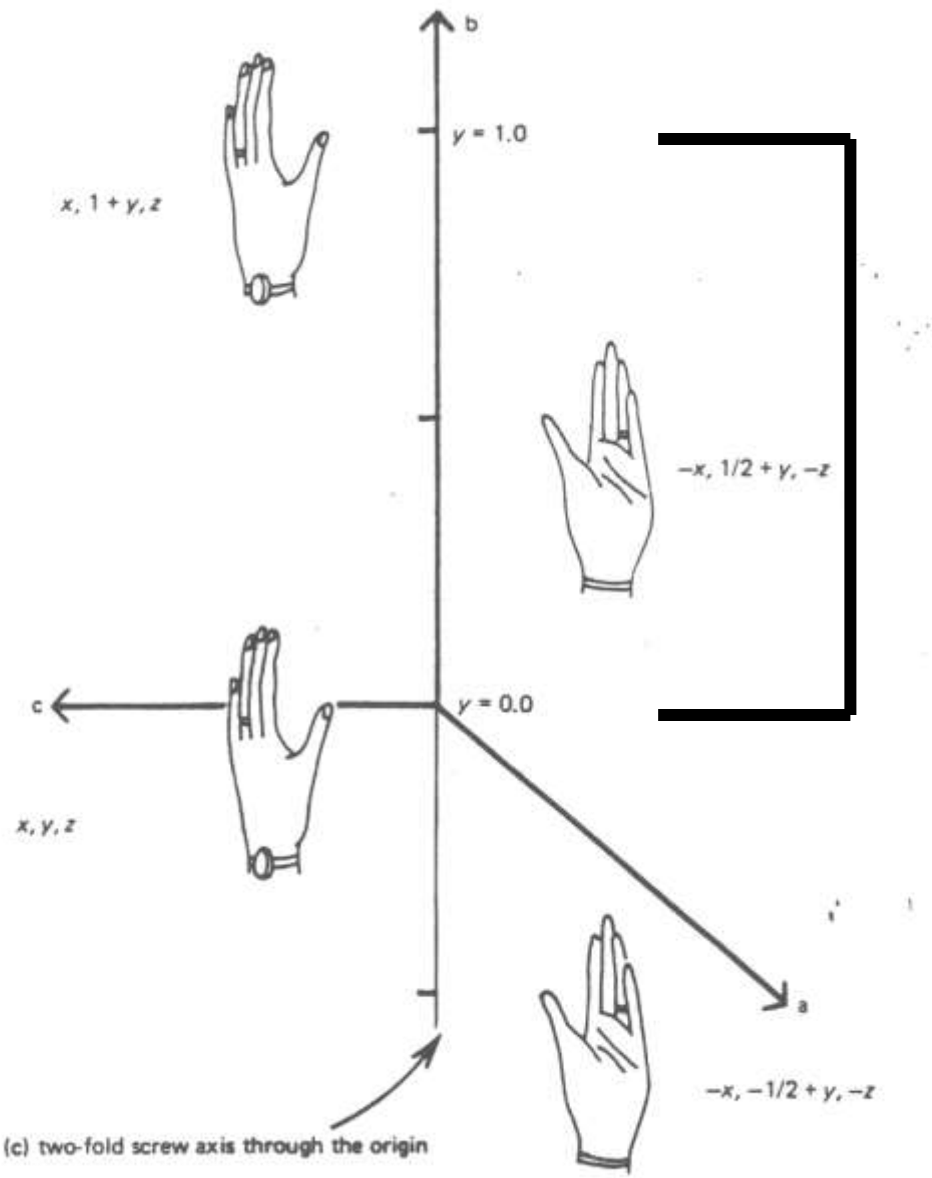
Screw Axes
(rotation + translation)

2-fold screw
180° + 1/2

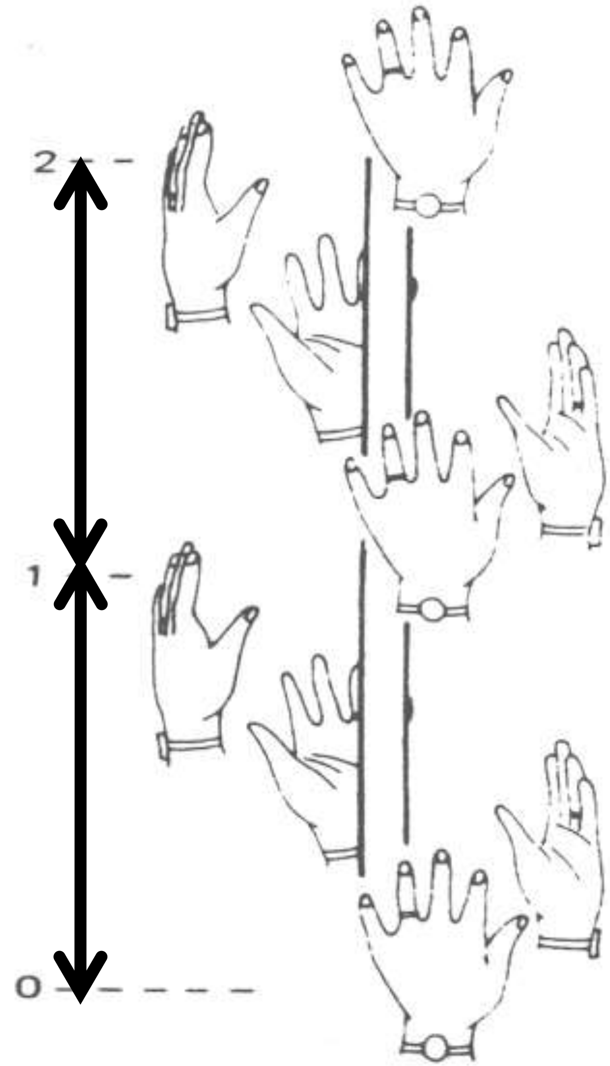
3-fold screw
120° + 1/3

4-fold screw
90° + 1/4

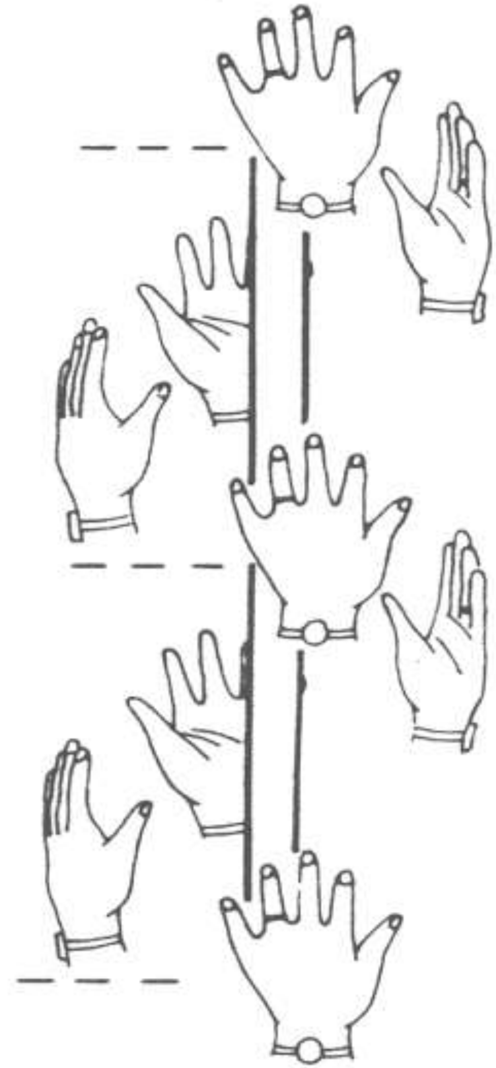
6-fold screw
60° + 1/6



4_1 and 4_3 Screw Axis



(d) 4_1 on left hand



4_3 on left hand

We will only look at examples having only 2-fold (2) or 2-fold screw (2_1) axes.

Unit Cell Selection is Based on Symmetry

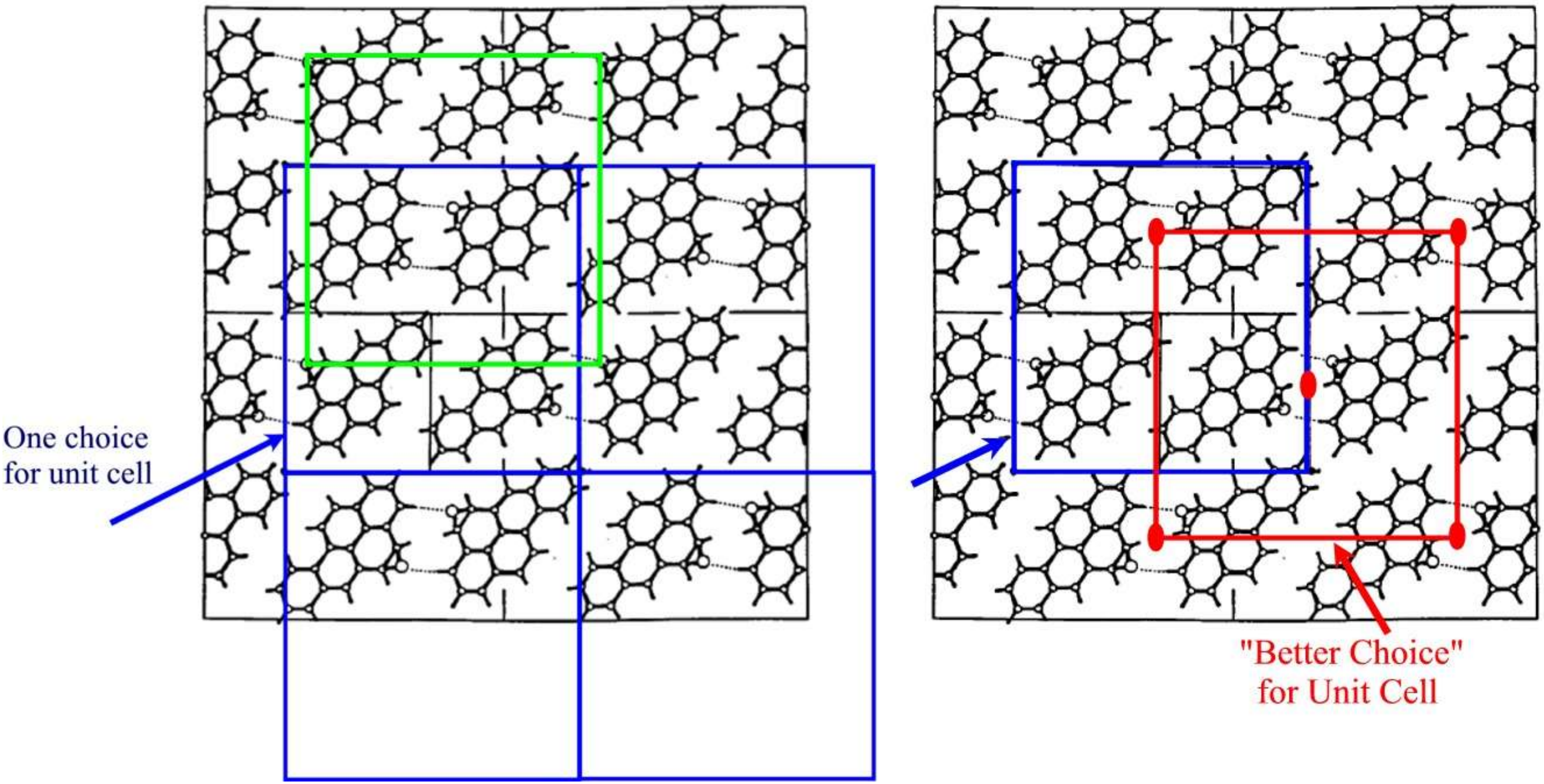
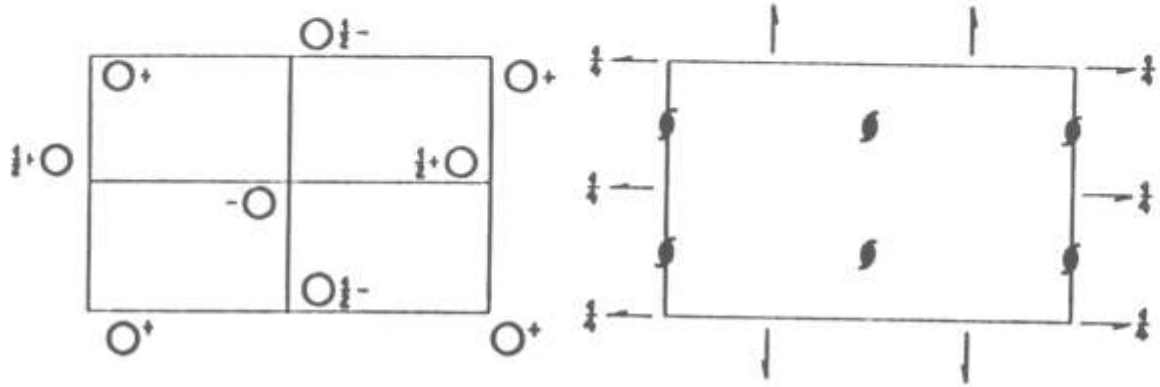


TABLE 16-5 *The 65 "Biological" Space Groups*

CRYSTAL SYSTEM	LATTICE	MINIMUM SYMMETRY OF UNIT CELL	UNIT CELL EDGES AND ANGLES[a]	DIFFRACTION PATTERN SYMMETRY[b]	SPACE GROUPS[c]
Triclinic	P	None	$a \neq b \neq c$	$\bar{1}$	$P1$
			$\alpha \neq \beta \neq \gamma$		
Monoclinic	P	2-fold axis parallel to **b**	$a \neq b \neq c$	$2/m$	$P2$, $P2_1$
	C		$\alpha = \gamma = 90°$		$C2$
			$\beta \neq 90°$		
Orthorhombic	P	3 mutually perpendicular 2-fold axes	$a \neq b \neq c$	mmm	$P222$, $P2_12_12_1$, $P222_1$, $P2_12_12$
	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		$\alpha = \beta = \gamma = 90°$		$I4$, $I4_1$
				$4/mmm$	$P422$, $(P4_122, P4_322)$, $P4_222$
					$P42_12$, $(P4_12_12, P4_32_12)$, $P4_22_12$
					$I422$, $I4_122$
Trigonal/rhombohedral	R[d]	3-fold axis parallel to **c**	$a = b = c$	$\bar{3}$	$R3$
	P[d]		$\alpha = \beta = \gamma \neq 90°$		$P3$, $(P3_1, P3_2)$
				$\bar{3}m$	$R32$
					$[P321, P312]$
					$[(P3_121, P3_221), (P3_112, P3_212)]$
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				$F23$
				$m3m$	$P432$, $(P4_132, P4_332)$
					$P4_232$
					$I432$, $I4_132$
					$F432$, $F4_132$

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
				0kl: No conditions
				h0l: No conditions
				hk0: No conditions
				h00: $h=2n$
				0k0: $k=2n$
				00l: $l=2n$

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.

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ymmetric Unit