Crystallography

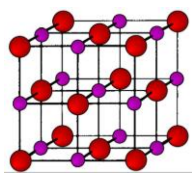
Topics:

1. **Image Formation** *(what we see is not always accurate)*
   - **Resolution / Wavelength (Amplitude, Phase) / Diffraction & Interference**
   - **Light Microscopy / EM / X-ray / (NMR)**
2. **Protein Data Bank (PDB)**
   - **Data mining and Protein Structure Analysis Tools**
3. **IYCr 2014 - Celebrating 100 years of X-ray Crystallography**
4. **X-Ray Crystallography – practical aspects**
   - **a) 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**

Crystallography – Worlds of Wonder

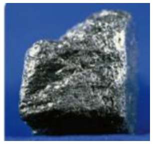
- **Crystallography - What is it? How does it Work?**
  - **Early Years – historical overview**
  - **Demonstration of diffraction / image formation**
  - **Crystals + X-rays → *record of Nobel Prizes***
- **Benefits of Crystallography to Society / IYCr 2014**
  - ***Crystallographic Awareness / Celebration / Training***
  - ***IYCr: Summits (Africa / Asia / Latin America)***
  - ***Crystal growth contests / Exhibits / etc.***
  - ***Crystallography Discovery Kit for teachers & museums***
  - ***symmetry / crystal growth / diffraction***

Chemistry / Bonding

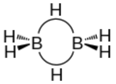


Sodium Chloride (NaCl) (a.k.a. Table salt)

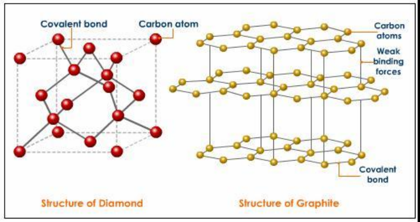
diamond
***Fd*–3m**
Non-conductor



graphite
***P*6$_3$/mmc**
Conductor



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

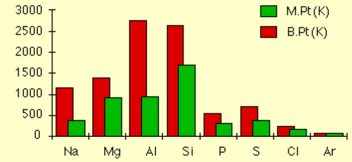


Semiconductors

Silicon - a giant covalent structure

Variation in physical properties in period 3

Melting and boiling points



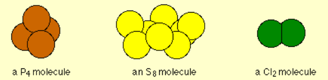
Silicon looks like a metal, but is a non-metal with the same structure as diamond. **Silicon is a semi-conductor.**

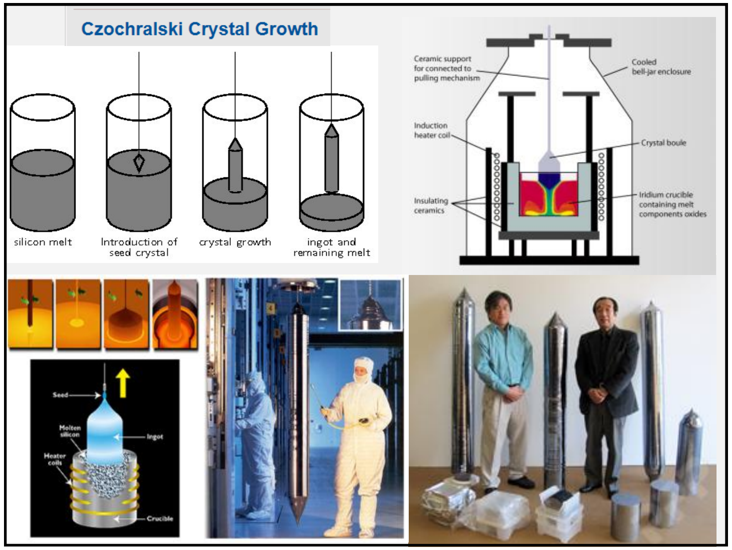
You can turn silicon into a **conductor** by **doping** it - mixing a small amount of an **impurity** into the silicon crystal.

Four molecular elements

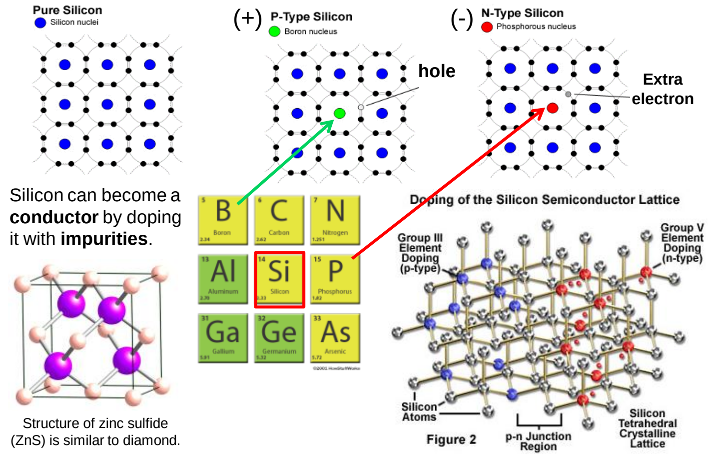
Phosphorus, sulphur, chlorine and argon are simple molecular substances with only van der Waals attractions between the molecules. Their melting or boiling points will be lower than those of the first four members of the period which have giant structures. The presence of individual molecules prevents any possibility of electrons flowing, and so none of them conduct electricity.

The sizes of the melting and boiling points are governed entirely by the sizes of the molecules:





Transistors - tiny switches that can be triggered by electric signals. They are the basic building blocks of microchips (PNP/NPN).

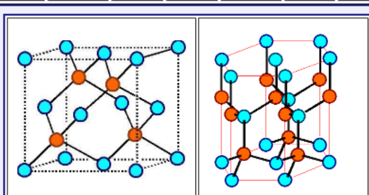


Silicon can become a **conductor** by doping it with **impurities**.

Structure of zinc sulfide (ZnS) is similar to diamond.

Basic Semiconductor Crystal Structure

Properties	Si	GaAs	InP	GaP	GaN	$In_{0,53}Ga_{0,47}As$
Band gap [eV]	1,12	1,42	1,35	2,26	3.39	0,75
Type	Indirect	Direct	Direct	Indirect	Direct	Direct
Lattice	fcc	fcc	fcc	fcc	hex	fcc



Zinc blende or sphalerite or Diamond structure

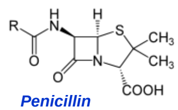
Wurtzite or hexagonal structure
Red lines are not showing bonds.

Wurtzite is the name of the **b-ZnS** modification - the hexagonal high-temperature variant. The named after the French chemist C. A. **Wurtz** (*** 1817, † 1884**),

Materials Research

Crystallography underpins the development of practically all new materials, from everyday products like computer memory cards to flat television screens, cars and airplane components. **Crystallographers not only study the structure of materials but can also use this knowledge to modify a structure to give it new properties** or to make it behave differently. The crystallographer can also establish the new **material's 'fingerprint'**. A company can then use this 'fingerprint' to prove that the new substance is unique when applying for a patent.

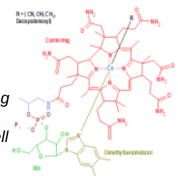
Crystallography helps to determine the ideal **combination of aluminum and magnesium** in alloys used in airplane manufacture. Too much aluminum and the plane will be too heavy, too much magnesium and it will be more flammable.



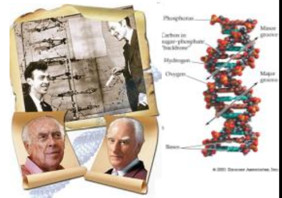
Penicillin

Medicine

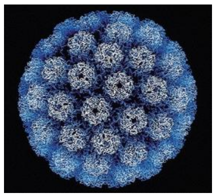
Penicillin kills bacteria by interfering with aminopetidase, an enzyme responsible for making bacteria cell wall. Human and mammals do not have this enzyme.



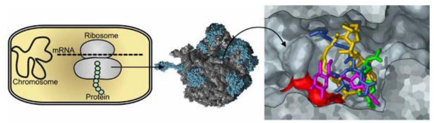
Vitamin B12

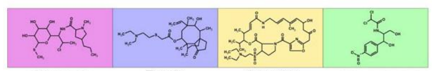


Structure of DNA – human genome, genetic diseases



SV40 (simian virus) structure, has been linked to mesothelioma.





Clindamycin | Tiamulin | Dalfopristin | Chloramphenicol

Chloramphenicol, tiamulin and other antibiotics target the peptidyl transferase center (PTC) on the bacterial ribosome.
Birte Vester Denmark

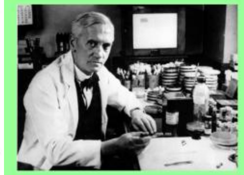
The Nobel Prize in Physiology or Medicine 1945
Sir Alexander Fleming, Ernst B. Chain, Sir Howard Florey

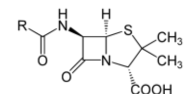
The Nobel Prize in Physiology or Medicine 1945

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?

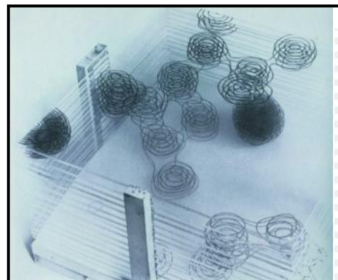


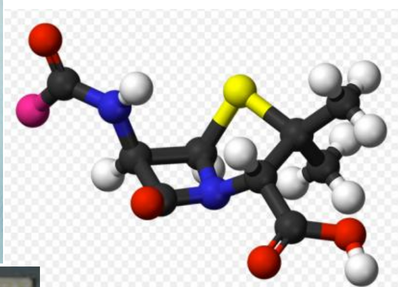


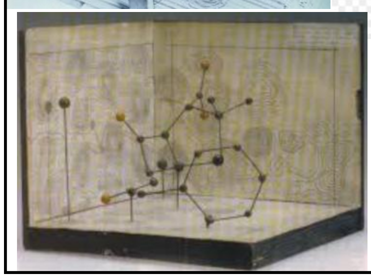
Penicillin

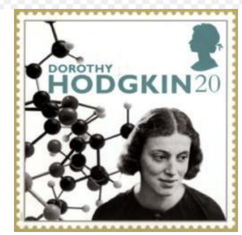
Brief History of Penicillin

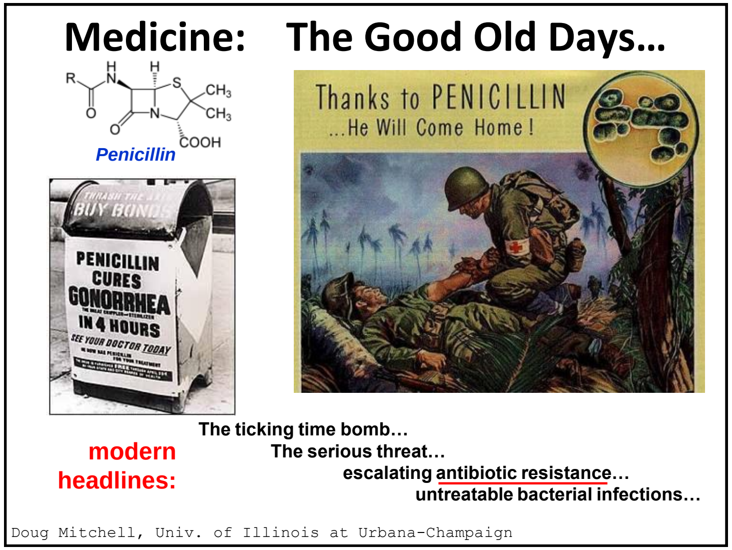
- **Alexander Fleming** (Scottish scientist) fought in **World War I**. His battlefront experience showed him how dangerous bacteria could be to human life. After the war he focused on finding a chemical that would stop bacterial infection.
- In the **Fall of 1928**, Fleming had prepared ***Staphylococcus*** 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 particular mold strain (later identified to be ***Penicillium notatum***) was a **good producer of penicillin**.
- In 1935, **Howard Florey** working on penicillin. 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**".
- **The first batches of this new wonder drug** became available in **1943** and were reserved for military use. **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.**

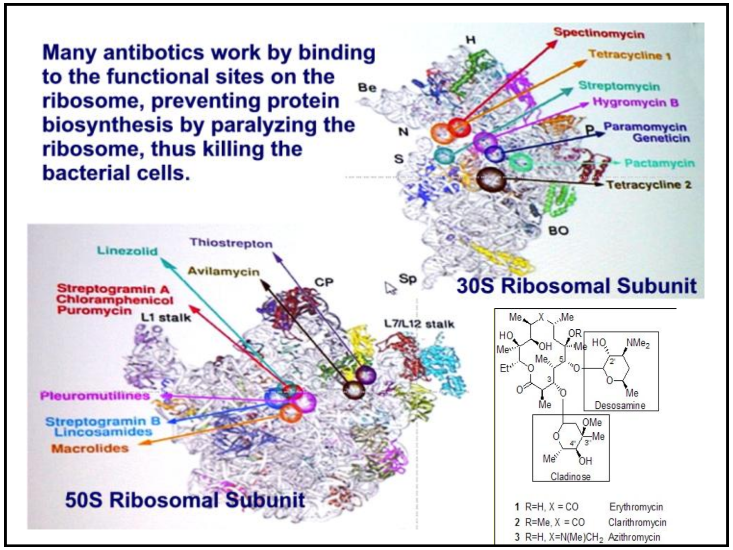


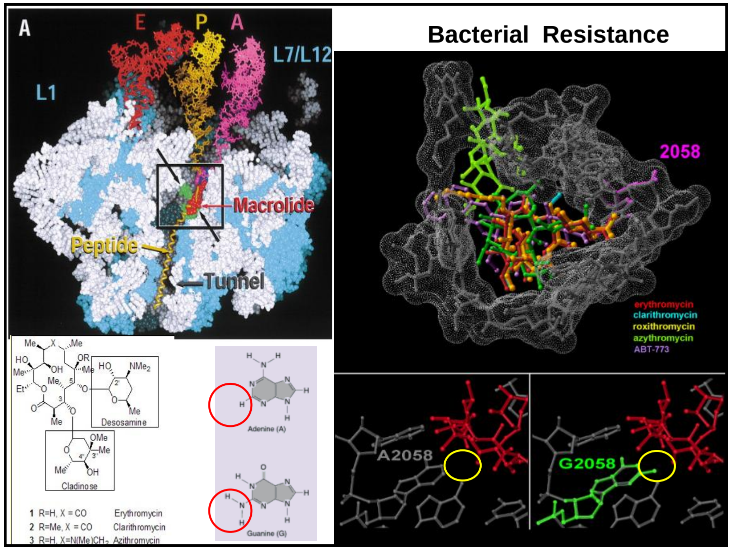


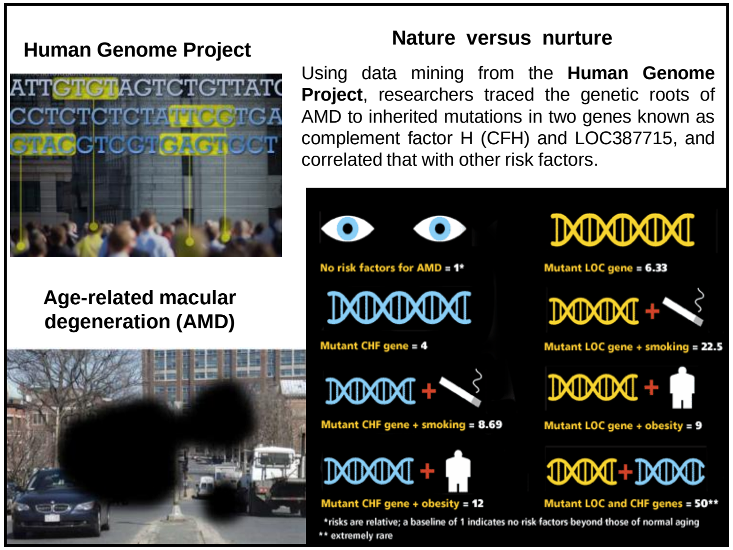





Medicine: The Good Old Days…
Penicillin
Thanks to PENICILLIN
…He Will Come Home!
PENICILLIN CURES GONORRHEA IN 4 HOURS
SEE YOUR DOCTOR TODAY
BUY BONDS
modern headlines:
The ticking time bomb…
The serious threat…
escalating antibiotic resistance…
untreatable bacterial infections…
Doug Mitchell, Univ. of Illinois at Urbana-Champaign

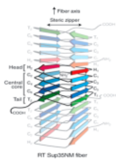

Many antibotics work by binding to the functional sites on the ribosome, preventing protein biosynthesis by paralyzing the ribosome, thus killing the bacterial cells.
Spectinomycin
Tetracycline 1
Streptomycin
Hygromycin B
Paramomycin
Geneticin
Pactamycin
Tetracycline 2
30S Ribosomal Subunit
Linezolid
Thiostrepton
Avilamycin
Streptogramin A
Chloramphenicol
Puromycin
L1 stalk
CP
L7/L12 stalk
Pleuromutilines
Streptogramin B
Lincosamides
Macrolides
50S Ribosomal Subunit
Desosamine
Cladinose
1 R=H, X = CO Erythromycin
2 R=Me, X = CO Clarithromycin
3 R=H, X=N(Me)CH2 Azithromycin


Bacterial Resistance
A
E P A
L1
L7/L12
Macrolide
Peptide
Tunnel
2058
erythromycin
clarithromycin
roxithromycin
azythromycin
ABT-773
Desosamine
Cladinose
1 R=H, X = CO Erythromycin
2 R=Me, X = CO Clarithromycin
3 R=H, X=N(Me)CH2 Azithromycin
Adenine (A)
Guanine (G)
A2058
G2058


Human Genome Project
Nature versus nurture
Using data mining from the Human Genome Project, researchers traced the genetic roots of AMD to inherited mutations in two genes known as complement factor H (CFH) and LOC387715, and correlated that with other risk factors.
Age-related macular degeneration (AMD)
No risk factors for AMD = 1*
Mutant LOC gene = 6.33
Mutant CHF gene = 4
Mutant LOC gene + smoking = 22.5
Mutant CHF gene + smoking = 8.69
Mutant LOC gene + obesity = 9
Mutant CHF gene + obesity = 12
Mutant LOC and CHF genes = 50**
*risks are relative; a baseline of 1 indicates no risk factors beyond those of normal aging
** extremely rare

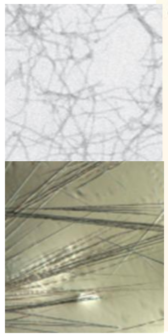
Amyloid Related Conditions

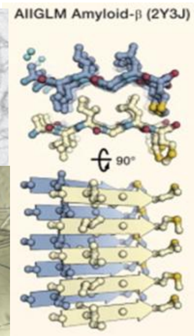
Amyloid (disease / protein)	**Prion (transmissible)** (disease / protein)	**Amyloid-like** (disease / protein)
Alzheimer's / Tau	Creutzfeldt-Jakob / PrP	Parkinson's / a-synuclein
Diabetes II / Amylin	Mad Cow / PrP	LouGehrig's / SOD



Steric Zipper Hypothesis:

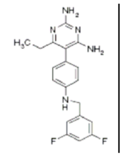
- >120 segments of amyloid-forming proteins form micro-crystals with a common flat sheet structural motif.
- Zipper-forming segments can seed parent proteins into fibers
- **Amyloid-inhibitors are designed to block steric zipper fibers**

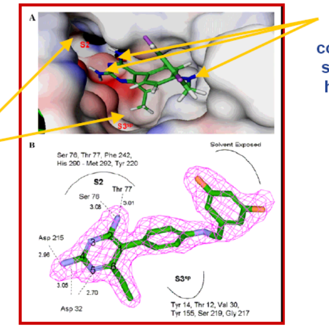




Crystallography in Drug Design

Renin inhibitors are a group of pharmaceutical drugs used primarily in treatment of hypertension (high blood pressure). The binding orientation of a lead compound to inhibit Renin was determined by X-ray crystallography.



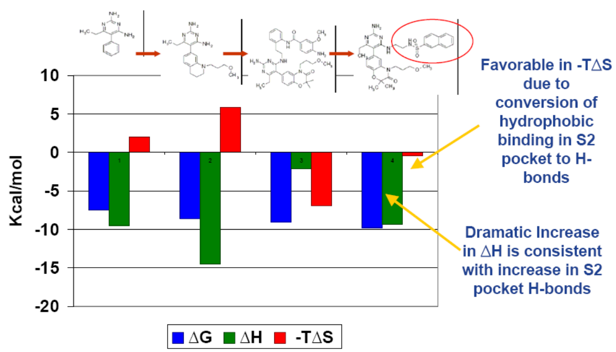


The unoccupied hydrophobic S2 and S3 pockets are opportunities to enhance favorable ΔS

favorable ΔH is consistent with the strong network of hydrogen bonds.

Crystallography in Drug Design

Renin inhibitors: Chemists use the information from the X-ray structure to improve binding of the lead compound. Modeling suggests substituting the aryl-benzamide with an aryl-sulfonamide to improve H-bonding to improve its fit on the target.



Favorable in -TΔS due to conversion of hydrophobic binding in S2 pocket to H-bonds

Dramatic Increase in ΔH is consistent with increase in S2 pocket H-bonds

Renin Inhibitor Binding Affinity Improved from 3.6×10^{-6} M to 79×10^{-9} M (46X)

Improved binding means less of the drug is needed, resulting in lower manufacturing costs per dose and a reduction of side effects.

- S3 Pocket – Ether addition improved enthalpy due to van der Waals bonds
- S2 Pocket – Aryl-Sulfonamide improved binding enthalpy while retaining hydrophobic advantage

imagination at work

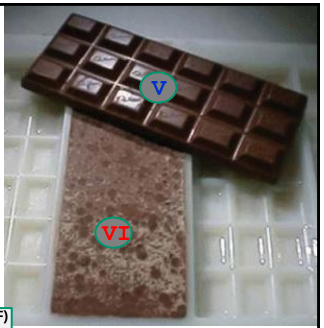
Space Exploration

*The **Curiosity rover** used X-ray crystallography in October 2012 to analyze soil samples on the planet **Mars**!*

NASA had equipped the rover with a diffractometer. The results suggested that the Martian soil sample was similar to the weathered basaltic soils of Hawaiian volcanoes.

Photo: NASA

Crystallography and Chocolate



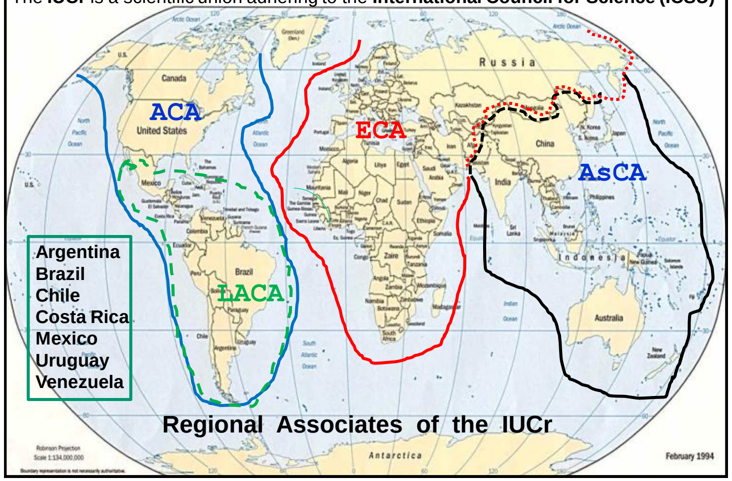
***Cocoa butter**, the most important ingredient of chocolate, **crystallizes in six different forms** but only one (form V) melts pleasantly in the mouth and has the surface sheen and crisp hardness that make it so tasty.*

Crystal form	Formation conditions	m. p. [°C]	
I	rapid cooling of the melt	17.3	
II	rapid cooling of the melt at 2 °C/min	23.3	
III	crystallization of the melt at 5–10 °C, converts into II at 5–10 °C	25.5	
IV	crystallization at 16–21 °C	27.3	
V *	slow crystallization of the melt	33.8	(93 °F)
VI *	from form V after several months at RT	36.3	(98 °F)

Unfortunately, this 'tasty' crystal form is not very stable so it tends to convert into the more stable form (VI), which is dull, has a soft texture and melts only slowly in the mouth, producing a coarse and sandy sensation on the tongue. The conversion is slow, but if chocolate is stored for a long time or at a warm temperature, it can develop a 'bloom,' a white, filmy residue that results from recrystallization. Chocolate-makers thus have to use a sophisticated crystallization process to obtain the most desirable crystal form of cocoa butter in chocolate. Adding milk fat retards the conversion so that the V→VI transition is less often observed in milk chocolate!

IUCr - International Union of Crystallography

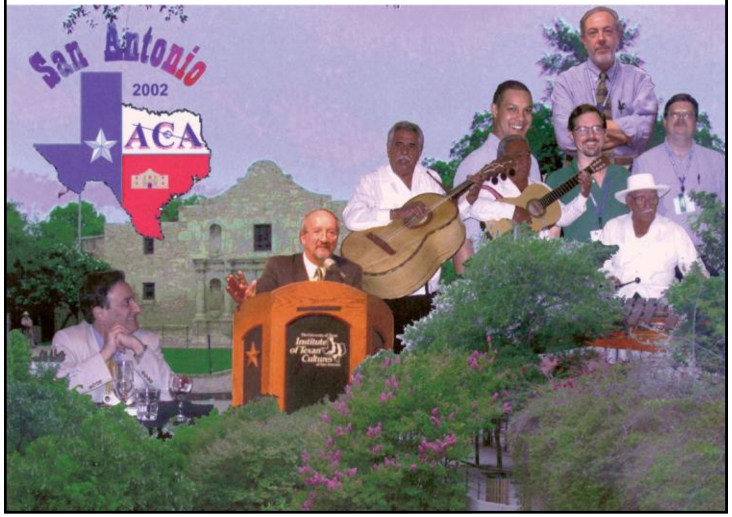
The **IUCr** is a scientific union adhering to the **International Council for Science (ICSU)**



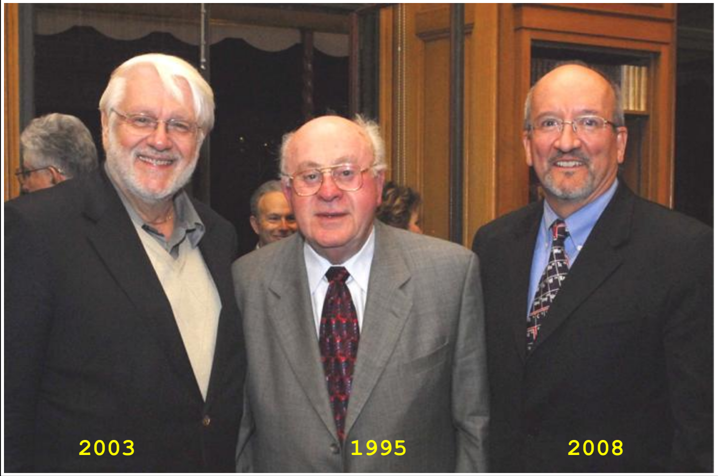
Each country is represented by it national committee – USNC/Cr

USNCCr - November 2001
Guest - Jack Marburger (White House Science Adviser, Dir. OSTP)

Regional Associates hold annual conferences - ACA Council



University of Texas at Austin – ACA Presidents



At the twenty third Congress and General Assembly of the International Union of Crystallography Professor Marvin L. Hackert was elected as the new President of the IUCr. The photograph shows the Convener of the Finance Committee and the Executive Secretary alongside Professor Hackert and the other members of the new Executive Committee for the triennium 2014-2017.

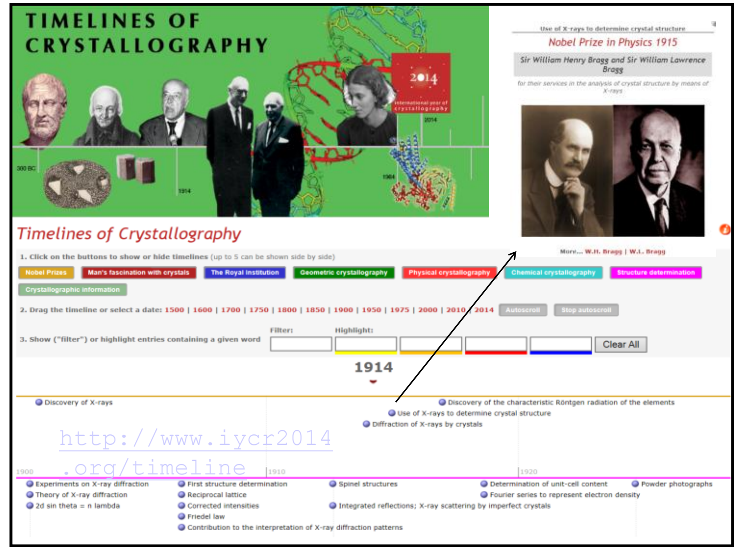
Back row: M. J. Cooper (Convener, IUCr Finance Committee), M. H. Dacombe (Executive Secretary). Executive Committee: J. M. Guss, R. Kuzel, M. Takata, W. Depmeier, S. Garcia-Granda. Front row: H. Dabkowska, L. Van Meervelt (General Secretary and Treasurer), M. L. Hackert (President), A. M. Glazer (Vice-President), G. R. Desiraju (Immediate Past President).

Please join the IUCr in welcoming the new Executive Committee and thanking those members retired.

The IUCr Intl. Congress 2014 - Montreal

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


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


TIMELINES OF CRYSTALLOGRAPHY
Nobel Prize in Physics 1915
Timelines of Crystallography
1914
Clear All
http://www.iycr2014.org/timeline


IUCr-UNESCO
OpenLab
OpenFactory
http://www.iycr2014.org/
bringing nations together
summit meetings
karachi
campinas
bloemfontein

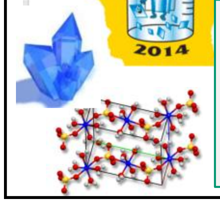

Latin American Summit - Campinas, Brazil September 22-24, 2012
pages.cnpem.br/iycr2014-lasummit
CNPEM
IYCr2014

Education / Celebration for IYCr 2014

Crystallography Discovery Kit for K-12 teachers / children's museums

i) Crystal Jars Kit

ii) Symmetry and Lattices

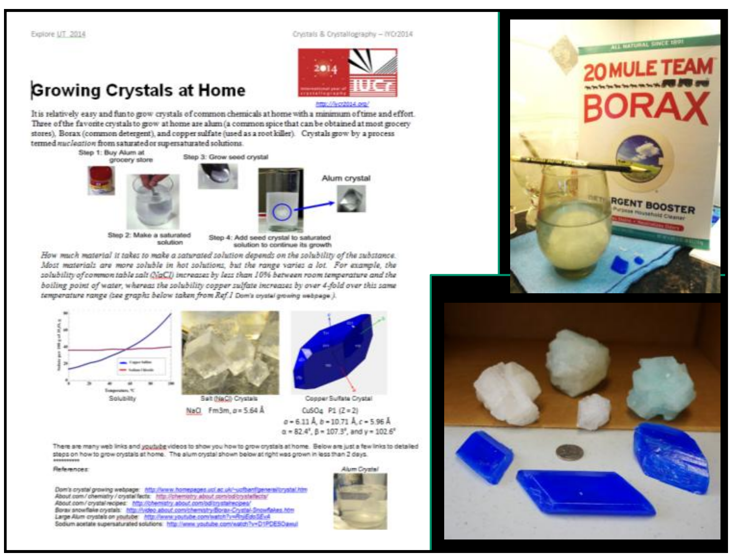


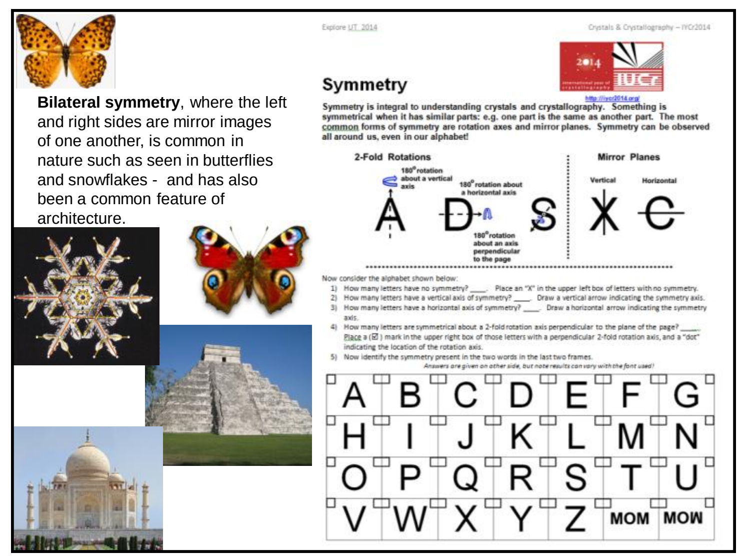
*For 2014 the material used for the crystal growing competition is cupric sulfate, **$CuSO_4.5H_2O$ (copper (II) sulfate pentahydrate**, or '**bluestone**').*

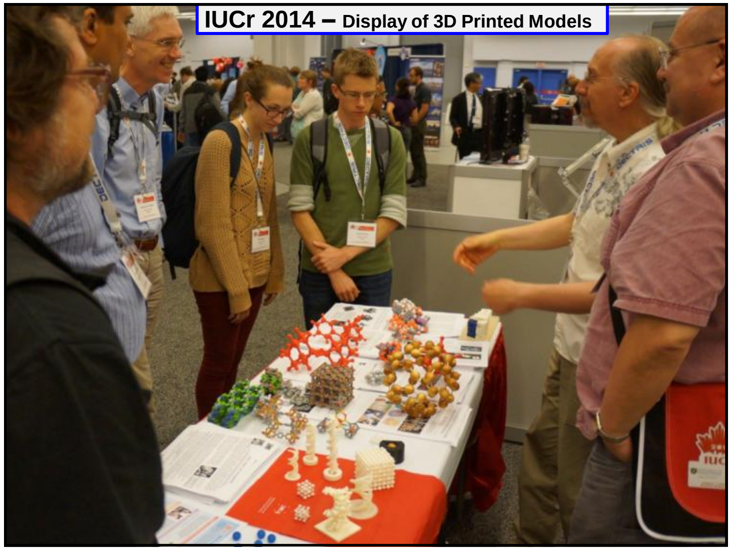
This material is chosen because it produces large beautiful blue crystals, which are neither too easy nor too difficult to grow. Cupric sulfate was also the compound used in the first X-ray diffraction experiment by Max von Laue in 1912.

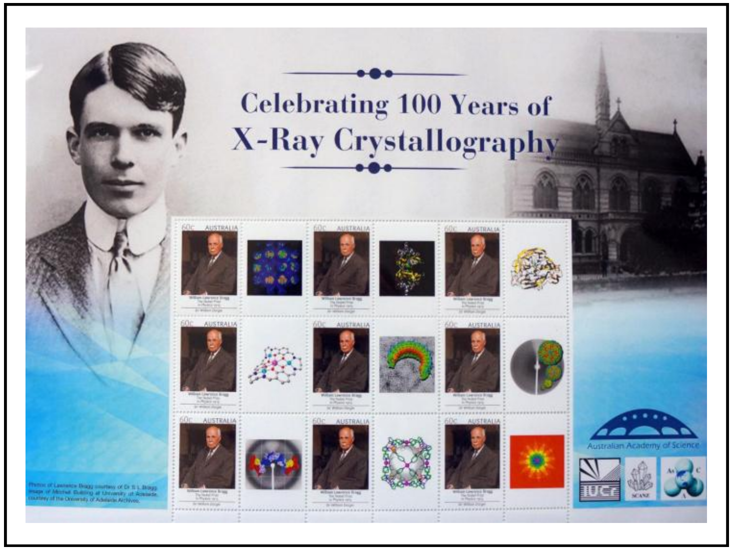
It is available free of charge on a first come first serve basis. Each participant or team is eligible for 200g of pure cupric sulfate.


What Starts Here Changes The World
THE UNIVERSITY OF TEXAS AT AUSTIN
General Information
Schedule
K-12 Connections
Promotional Resources
Media Gallery
Site Map
SAVE THE DATE: Saturday, March 1, 2014
EXPLORE UT
THE BIGGEST OPEN HOUSE IN TEXAS
Saturday, March 1, 2014
11 a.m. to 5 p.m.
Free. No registration required.

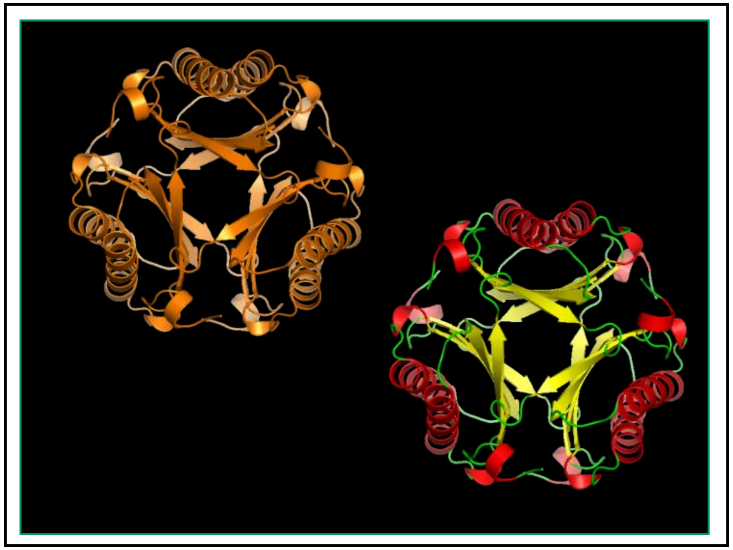

Explore UT 2014
Crystals & Crystallography – IYCr2014
Growing Crystals at Home
http://iycr2014.org/
It is relatively easy and fun to grow crystals of common chemicals at home with a minimum of time and effort. Three of the favorite crystals to grow at home are alum (a common spice that can be obtained at most grocery stores), Borax (common detergent), and copper sulfate (used as a root killer). Crystals grow by a process termed nucleation from saturated or supersaturated solutions.
Step 1: Buy Alum at grocery store
Step 2: Make a saturated solution
Step 3: Grow seed crystal
Step 4: Add seed crystal to saturated solution to continue its growth
Alum crystal
How much material it takes to make a saturated solution depends on the solubility of the substance. Most materials are more soluble in hot solutions, but the range varies a lot. For example, the solubility of common table salt (NaCl) increases by less than 10% between room temperature and the boiling point of water, whereas the solubility copper sulfate increases by over 4-fold over this same temperature range (see graphs below taken from Ref.1 Dom's crystal growing webpage.).
20 MULE TEAM
BORAX
DETERGENT BOOSTER

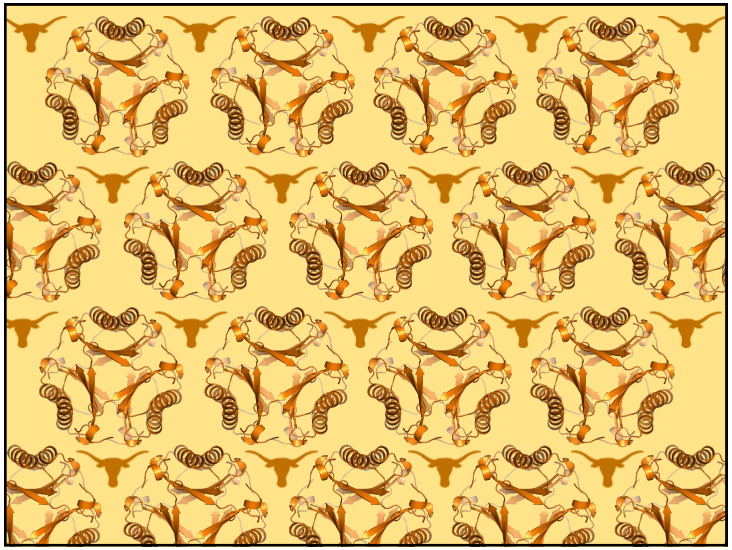

Bilateral symmetry, where the left and right sides are mirror images of one another, is common in nature such as seen in butterflies and snowflakes - and has also been a common feature of architecture.
Explore UT 2014
Crystals & Crystallography – IYCr2014
Symmetry
http://iycr2014.org/
Symmetry is integral to understanding crystals and crystallography. Something is symmetrical when it has similar parts: e.g. one part is the same as another part. The most common forms of symmetry are rotation axes and mirror planes. Symmetry can be observed all around us, even in our alphabet!
2-Fold Rotations
180° rotation about a vertical axis
180° rotation about a horizontal axis
180° rotation about an axis perpendicular to the page
Mirror Planes
Vertical
Horizontal
Now consider the alphabet shown below:
1) How many letters have no symmetry? ____. Place an "X" in the upper left box of letters with no symmetry.
2) How many letters have a vertical axis of symmetry? ____. Draw a vertical arrow indicating the symmetry axis.
3) How many letters have a horizontal axis of symmetry? ____. Draw a horizontal arrow indicating the symmetry axis.
4) How many letters are symmetrical about a 2-fold rotation axis perpendicular to the plane of the page? ____. Place a (☑) mark in the upper right box of those letters with a perpendicular 2-fold rotation axis, and a "dot" indicating the location of the rotation axis.
5) Now identify the symmetry present in the two words in the last two frames.
Answers are given on other side, but note results can vary with the font used!
A B C D E F G
H I J K L M N
O P Q R S T U
V W X Y Z MOM MOW


IUCr 2014 – Display of 3D Printed Models


Celebrating 100 Years of
X-Ray Crystallography
Australian Academy of Science
IUCr


HELVETIA 85
HELVETIA 100
SLOVENSKO
BHARAT INDIA
MOLDOVA
Turquoise
Emerald
Topaz
Carnelian
Jasper
Pinkmorganite
Amethyst
Zircon
Quartz
Lazurite
Aquamarine
Agate



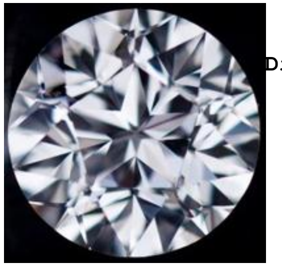


Crystallography

Topics:

1. **Image Formation** *(what we see is not always accurate)*
   Resolution / Wavelength (Amplitude, Phase) / Diffraction & Interference
   Light Microscopy / EM / X-ray / (NMR)
2. **Protein Data Bank (PDB)**
   Data mining and Protein Structure Analysis Tools
3. **IYCr 2014 - Celebrating 100 years of X-ray Crystallography**
4. **X-Ray Crystallography – practical aspects**
   - **a) 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**

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



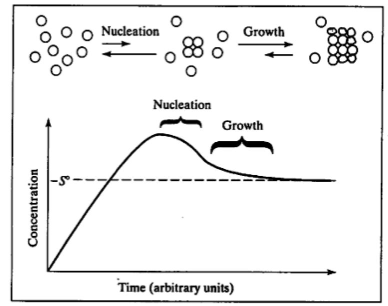
Diamond

Pink Diamond

Uncut Diamond

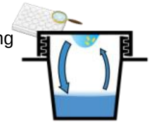
Crystals

Growing protein crystals.

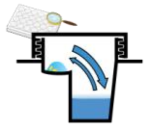


Methods to slowly change solution conditions

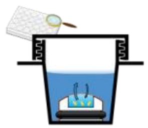
Hanging Drop



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

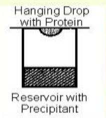
Methods for protein crystallization

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

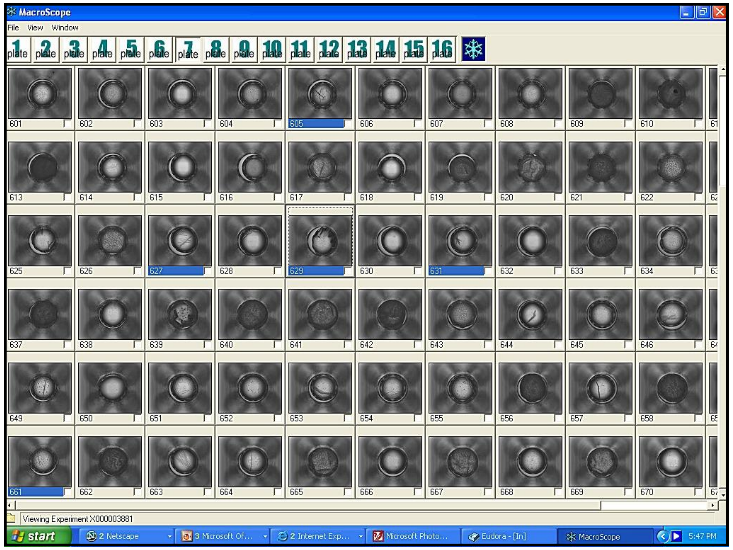
The Experimental Setup

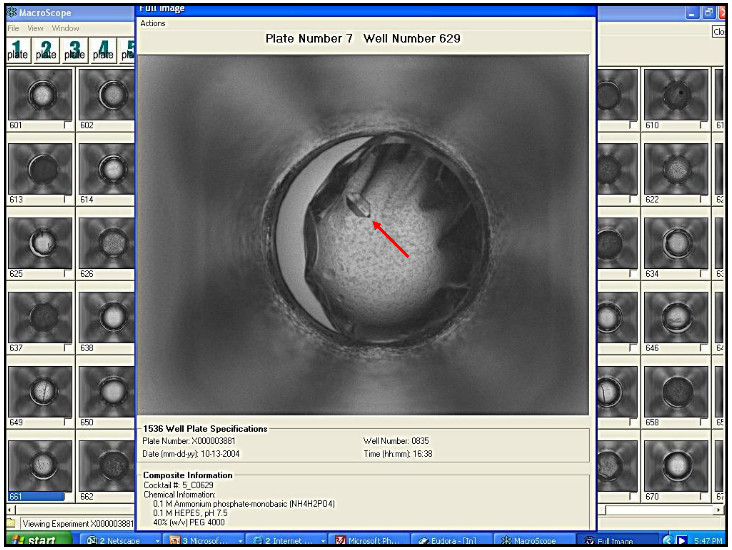
In order to obtain a crystal, the protein molecules must assemble into a periodic lattice. One starts with a solution of the protein with a fairly high concentration (2-50 mg/ml) and adds reagents that reduce the solubility close to spontaneous precipitation. By slow further concentration, and under 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.

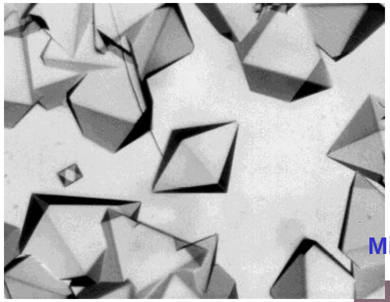


Hampton Crystal Screen Solutions

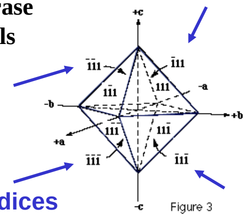
Tube #	SALT	BUFFER	Precipitant	Miniscreen	Tube #
1	0.02M Calcium Chloride	0.1M Na Acetate pH 4.6	30% w/v 2-methyl-2,4-pentanediol	Y	1
2	None	None	0.4M K,Na Tartrate tetrahydrate		2
3	None	None	0.4M Ammonium dihydrogen phosphate		3
4	None	0.1M Tris-HCl pH 8.5	2.0M Ammonium Sulfate	Y	4
5	0.2M tri-sodium 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% w/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



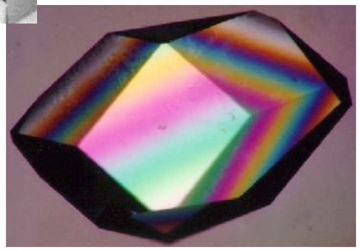




Glucose Isomerase Crystals



Miller Indices



Lysozyme Crystals

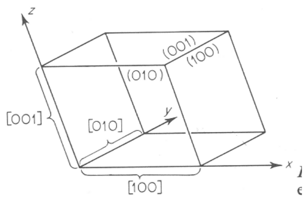
Bragg Planes

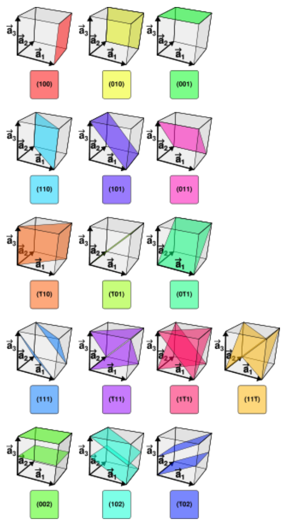
X-ray scattering can be understood as if the x-rays are reflected from planes in the crystal.

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

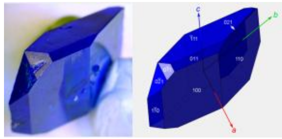
Miller indices are used to define the direction of planes within a crystal. A plane with Miller indices **h,k,l intersects the unit cell edges a, b, c at points a/h, b/k and c/l.**

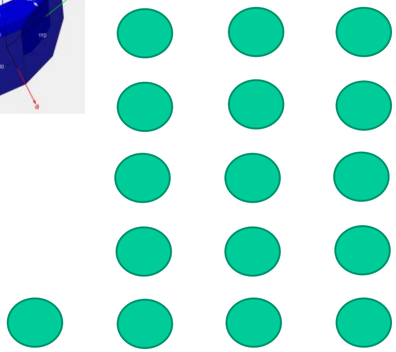
(3 integers define the direction of a plane).



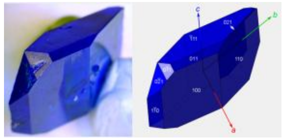


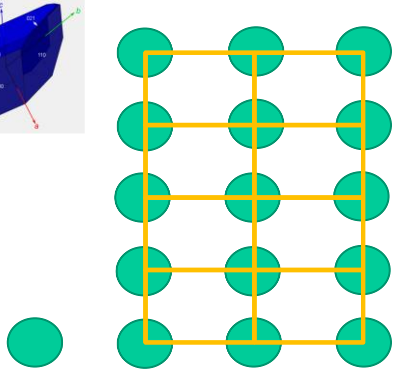
Atoms in space



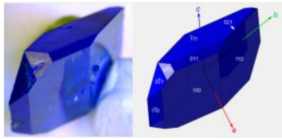


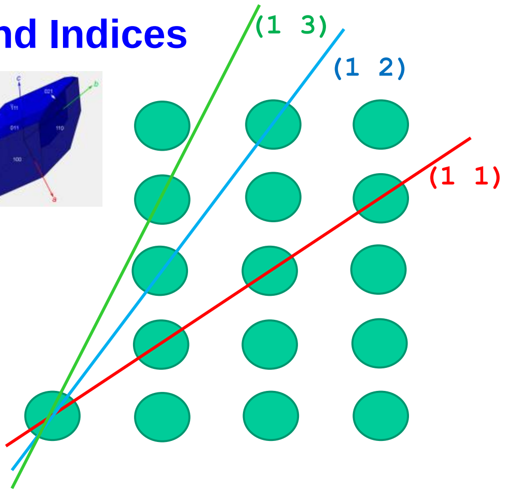
Atoms in space / Unit Cell



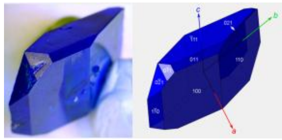


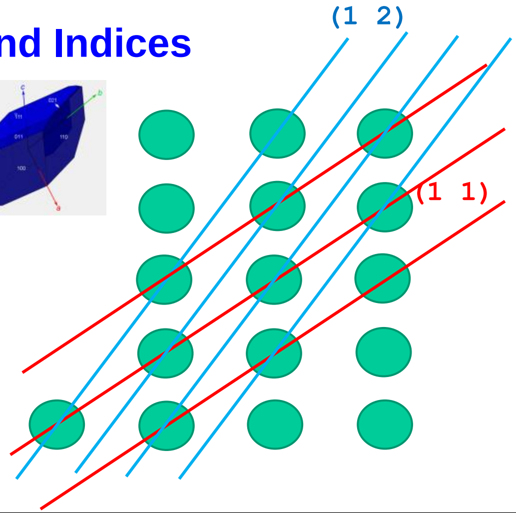
Planes and Indices



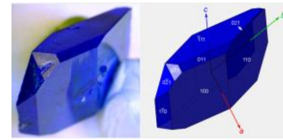


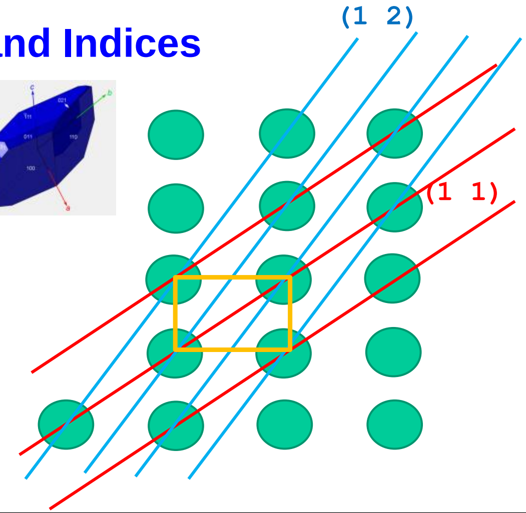
Planes and Indices



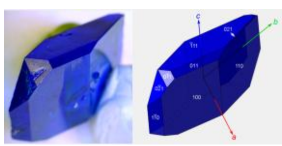


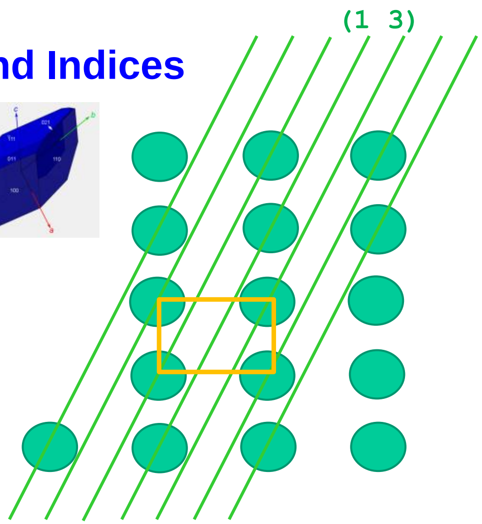
Planes and Indices





Planes and Indices





Name that Bragg “plane”

1 1 0 | 1 3 0 | 2 -1 0 (or -2 1 0)

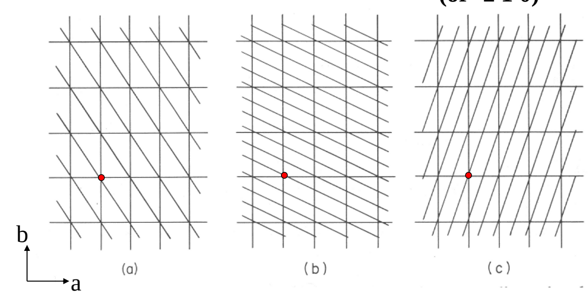
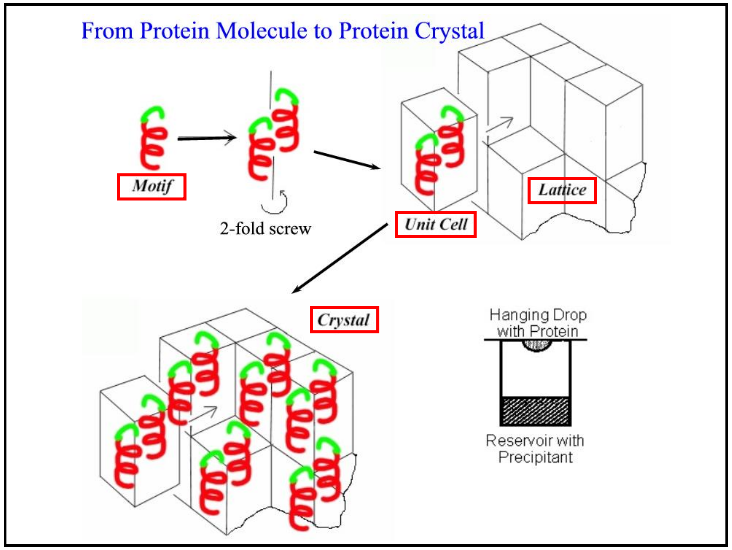
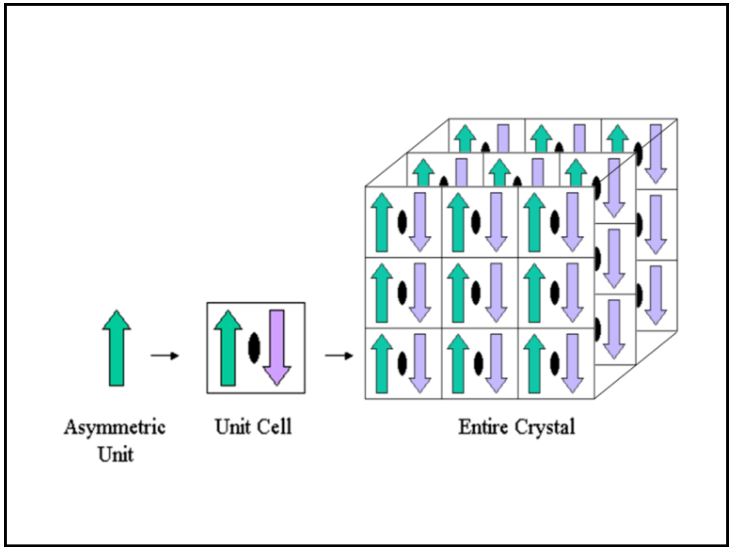


Figure 2.5. Three families of lattice "planes" in a two-dimensional lattice.


From Protein Molecule to Protein Crystal
Motif
2-fold screw
Unit Cell
Lattice
Crystal
Hanging Drop with Protein
Reservoir with Precipitant


Asymmetric Unit
Unit Cell
Entire Crystal