

We will start momentarily at 2pm ET



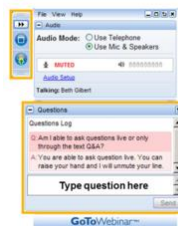
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<http://acswebinars.org/crystallography>

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## Have Questions?



### “Why am I muted?”

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Type them into questions box!

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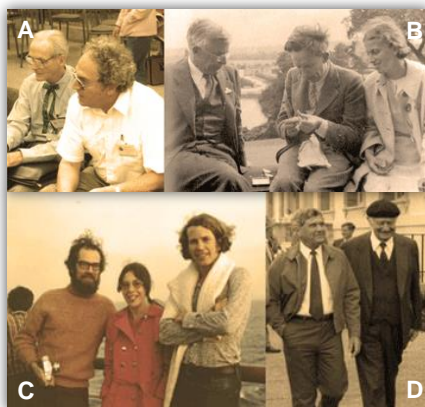


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- C) Walter Hamilton, Helen Berman, and Tom Koetzie on their way to a meeting in Aarhus in 1972.
- D) Richard E. Marsh and Linus Pauling, at Caltech during Pauling's 85th birthday celebration in 1986.

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## Fulbright Opportunities in 2015-16

May 15, 2014; 3:00pm EDT



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## Celebrate 2014, International Year of Crystallography!



Photo Credit: IYCR

<http://www.iycr2014.org/>

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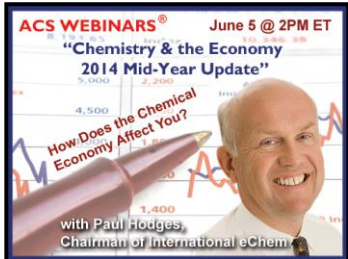
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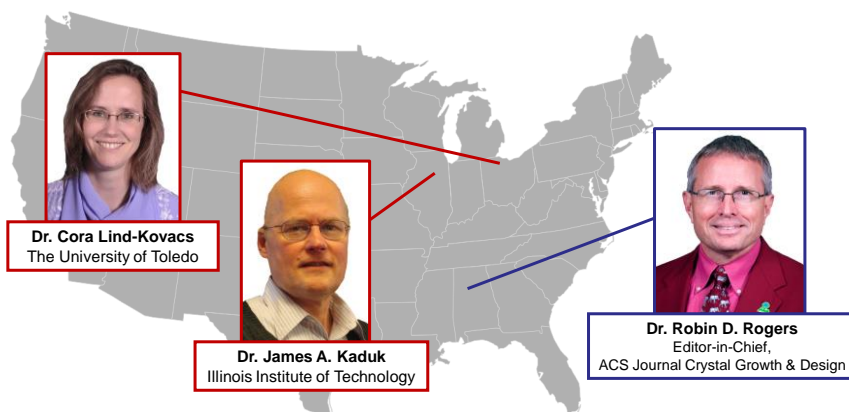
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***“Crystallography Frontiers:***  
*How Chemistry Reveals the Wonder of Everyday Materials”*



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## ***Crystallography Frontiers:***

*How Chemistry reveals the  
wonders of Everyday Materials*



Cora Lind-Kovacs  
Department of Chemistry & Biochemistry  
The University of Toledo  
Toledo, OH 43606  
[cora.lind@utoledo.edu](mailto:cora.lind@utoledo.edu)

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## Audience Survey:

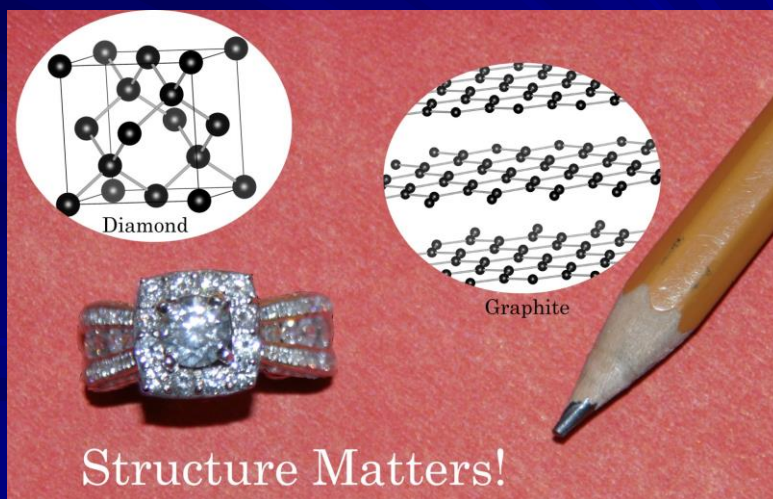
“Do you use crystallography in your work?”

- Yes, I carry out crystallographic experiments myself
- Kind of – I don’t do the experiments, but somebody else does crystallographic characterization for me
- No, I do not use any crystallography
- I can’t tell you, because I have no clue what crystallography is!

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## *Elemental Composition Is Not Enough*

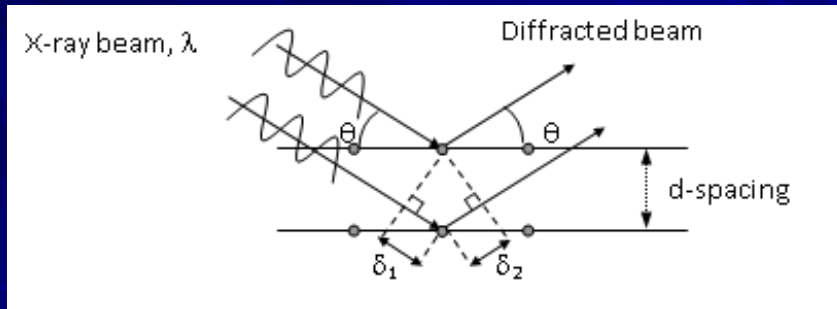
- It’s not just what’s in a compound – connectivity matters!
  - “Function follows form”



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## Determining the 3D Structure of Solids

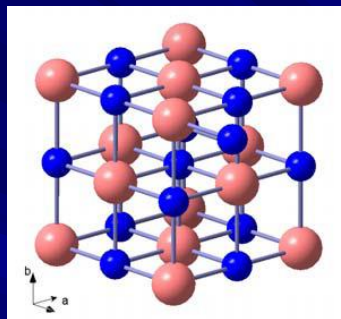
- Diffraction is often illustrated using Bragg's law
  - Not the full picture, but convenient and usually works!



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

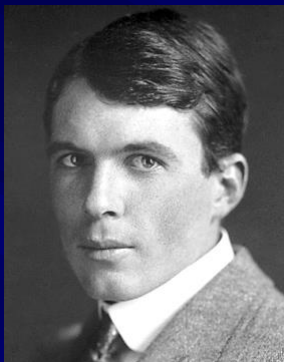
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## First Crystal Structures



- 1913: NaCl, KCl, KBr, diamond
- Structure of NaCl showed equally spaced Na and Cl atoms

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Sir William Lawrence Bragg

"In sodium chloride there appear to be no molecules represented by NaCl. The equality in number of sodium and chlorine atoms is arrived at by a chess-board pattern of these atoms; it is a result of geometry and not of a pairing-off of the atoms".

No molecules!

Admittedly, not everybody was happy to accept this...

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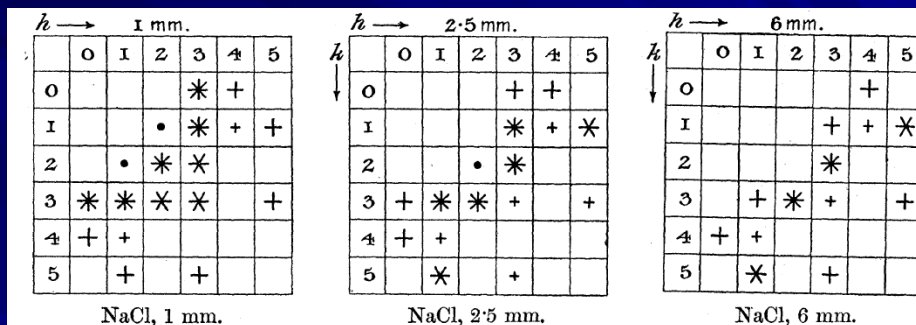
Henry E. Armstrong

"This statement is more than repugnant to common sense it is absurd to the  $n^{\text{th}}$  degree; not chemical cricket. Chemistry is neither chess nor geometry, whatever X-ray physics may be...It were time chemists took charge of chemistry once more and protected neophytes against the worship of false gods; at least taught them to ask for something more than chess-board evidence."

H. Armstrong, Nature, 1927, 120, p. 478

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## The Chess-Board Evidence



From: W.L. Bragg, "The Structure of Some Crystals as indicated by their Diffraction of X-rays." Proc. Roy. Soc. 89, 248-277.

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## Things we Take for Granted Concepts Illuminated By Crystallography

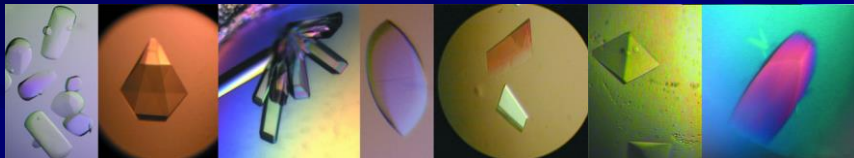


Photo Credit: <http://www.iycr2014.org/>

- The nature of atomic bonding
  - Ionic bonding, covalent bonding, metallic bonding, H-bonding
  - Multiple bonds versus single bonds; bond lengths
  - Resonance
  - Exotic bonds, e.g. 2-electron-3-center bonds, multiple metal bonds
- Molecular and extended structures

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## *Things we Take for Granted* *Concepts Illuminated By Crystallography*

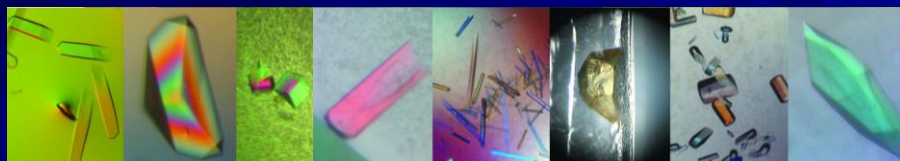


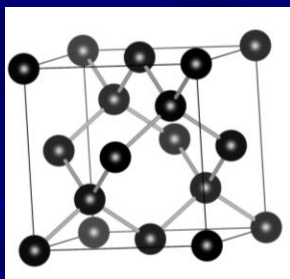
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- Polymorphism and implications on materials' properties
  - Inorganic solids
  - Drugs
- Biological structures
  - DNA, Enzymes, proteins, viruses, active sites...

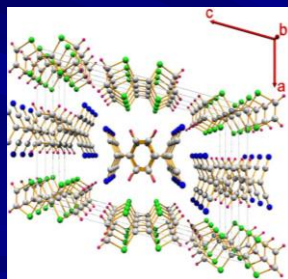
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## *Crystallography:* *Foundation of Modern Science and Engineering*

- We take knowledge of structure for granted and use it to explain and target properties all the time
  - Applies especially to theoreticians!



1913



1974



2000

26



## Audience Trivia Question:

### “What Happened Here?”

- Corrosion is everywhere – who put this metal bar into some corrosive solution?
- That looks pretty burned to me...
- Part of the metal bar has “frost bite”
- Violence is a problem even for metal bars - somebody took a hammer to it



www.periodictable.ru

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## Some Real Life Examples Where Structure Matters

- Tin pest destroyed many old organs and other pure tin compounds (buttons, coins, modern day solder...)
  - Can be avoided by adding impurities that stabilize metallic structure!



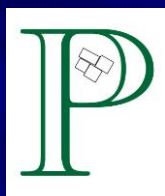
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[http://www.periodictable.ru/050Sn/Sn\\_en.html](http://www.periodictable.ru/050Sn/Sn_en.html)

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# *Understanding Everyday Materials using X-ray Powder Diffraction*



ILLINOIS INSTITUTE  
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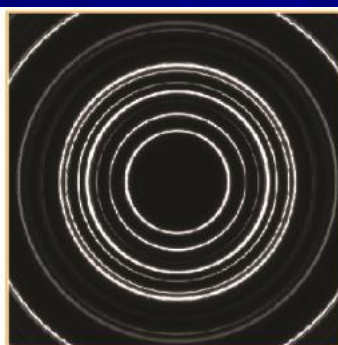
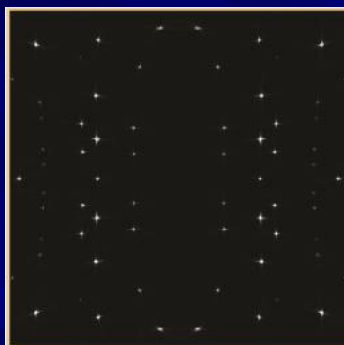
James A. Kaduk  
Illinois Institute of Technology  
Chicago IL 60616  
[kaduk@polycrystallography.com](mailto:kaduk@polycrystallography.com)

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## *X-ray Diffraction*

Single Crystal

Powder



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## Why do powder diffraction?

Real materials are not (usually) single crystals!

- Qualitative phase analysis
- Quantitative phase analysis
- Structure solution and refinement (Rietveld)
- Size/strain
- Texture
- *In situ*, time-resolved, *operando*, ...

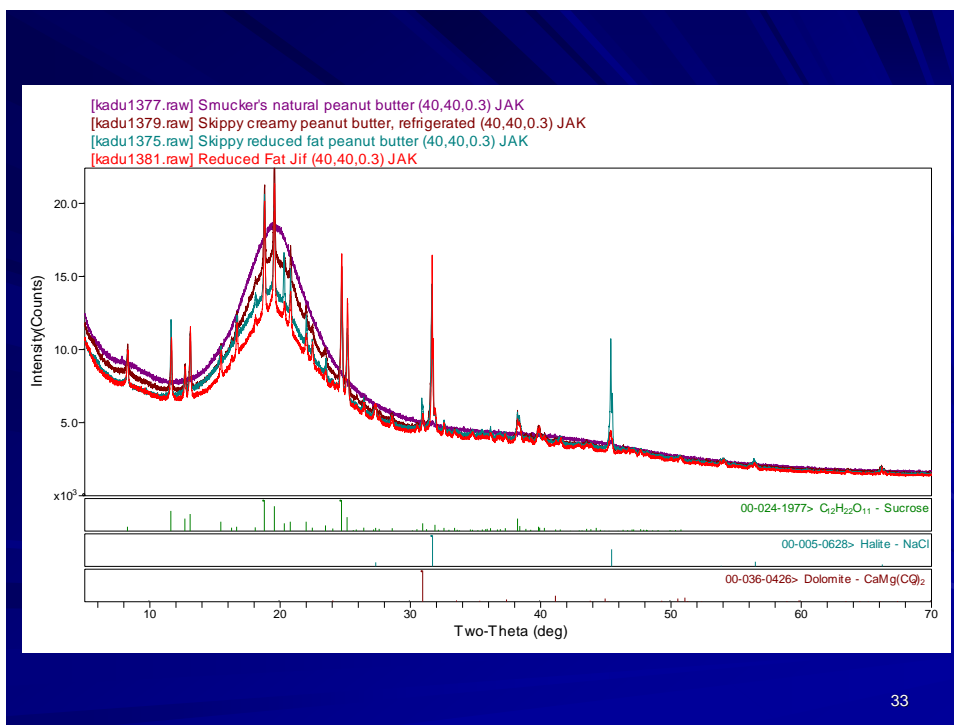
Question: Which of these would be important in your research/development project?

31

## Peanut Butter



32

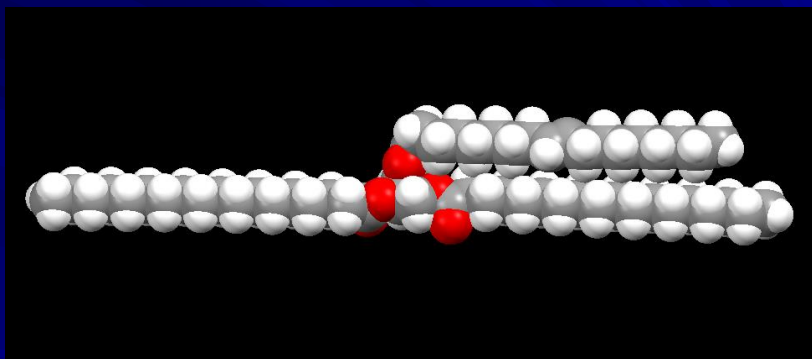


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Sample	Skippy Creamy	Skippy Reduced Fat	Jif Reduced Fat	Smucker's Natural
Ingredients	peanuts sugar salt hydr. veg. oils	peanuts corn syrup sol. sugar soy protein salt hydr. veg. oils mono/diglyc. minerals vitamins	peanuts corn syrup sol. sugar soy protein salt hydr. veg. oils molasses minerals vitamins	peanuts salt
sucrose, $C_{12}H_{22}O_{11}$ wt%	9.4	10.0	12.2	-
NI sugars, wt%	9.4	11.4	11.1	3.1
halite, NaCl wt%	~1	~2?	~1	Small
NI NaCl, wt%	1.2	1.2	1.6	1.0
dolomite, $CaMg(CO_3)_2$ wt%	-	0.2	-	-
$\beta_2$ fat, SSS wt%	-	-	1.4	-

34

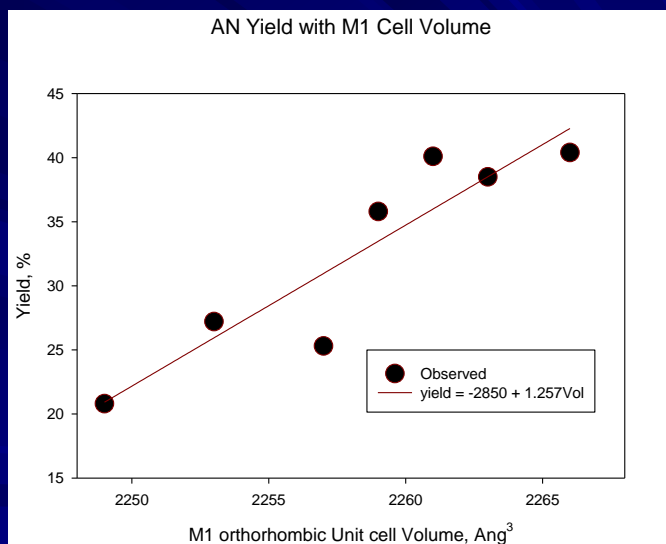
## Fat Molecule Structure



Determined in studies of chocolate!

35

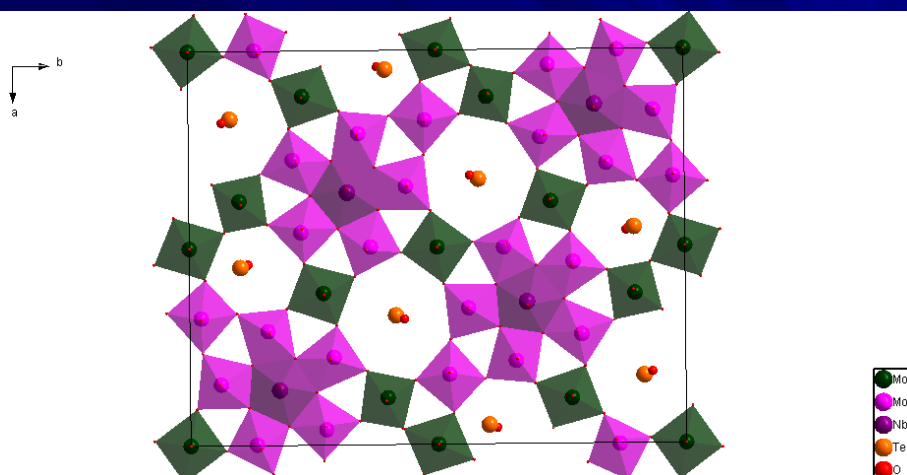
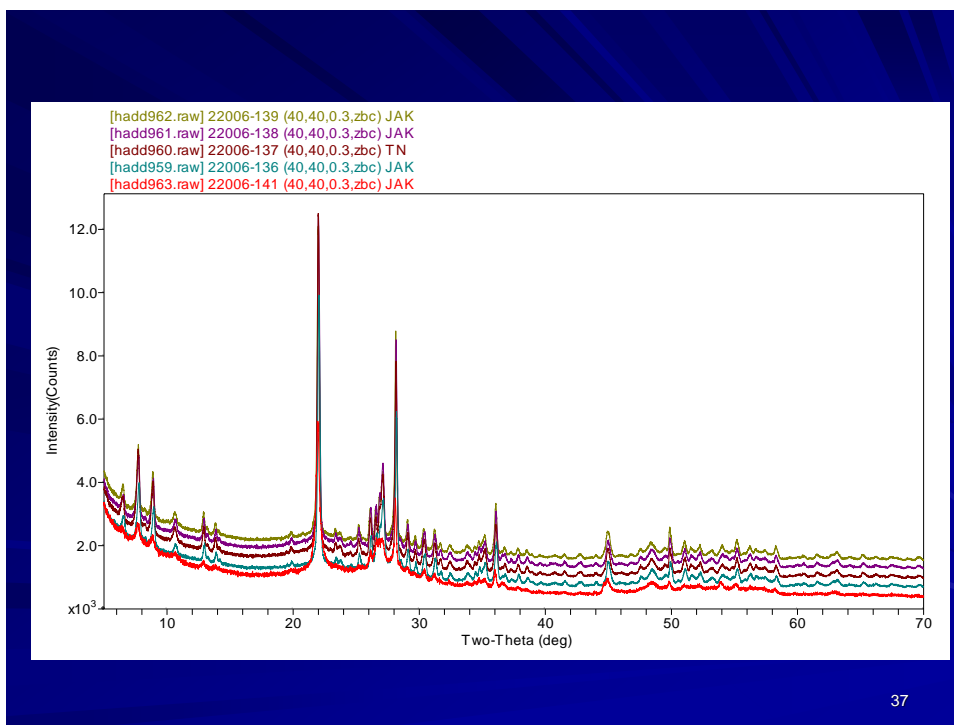
## Structure / Property Correlations



Propane Ammoxidation Catalysts

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## **US Patent 8,697,596** (*Ineos USA LLC*)

Claims on:

- Unit cell volume  $\sim 2250\text{-}2350 \text{ \AA}^3$
- Aspect ratio  $\sim 0.7\text{-}2.0$
- Composition ranges



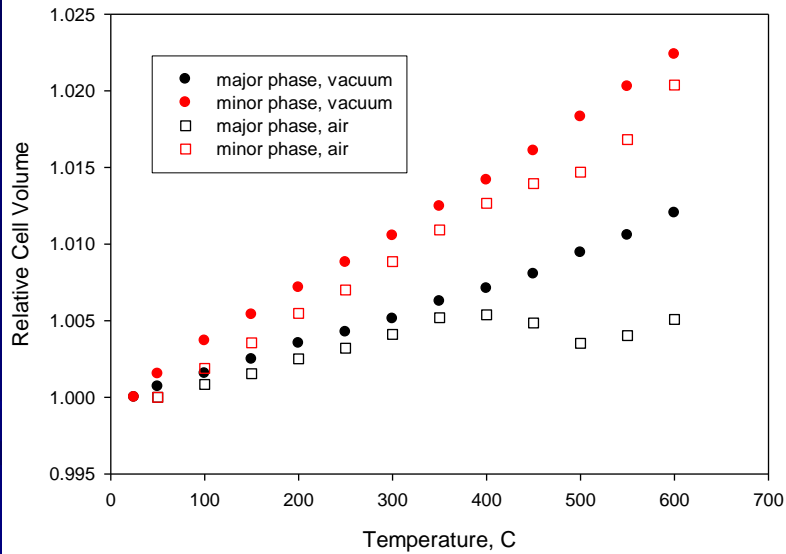
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**“Every** catalyst I have ever studied at/near reaction conditions has had a different structure than at ambient!”

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Thermal Expansion in  
21207-66-48 GL#2 2-18-08



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## Commercial Pharmaceuticals



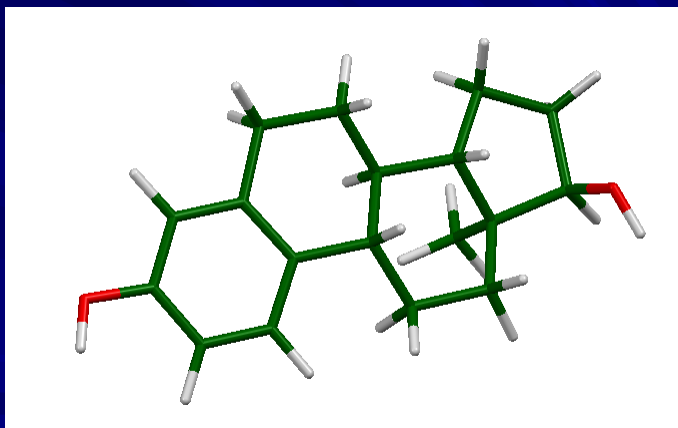
$17\alpha$ -Estradiol

Eli-Cranell Alpha, Pantosin

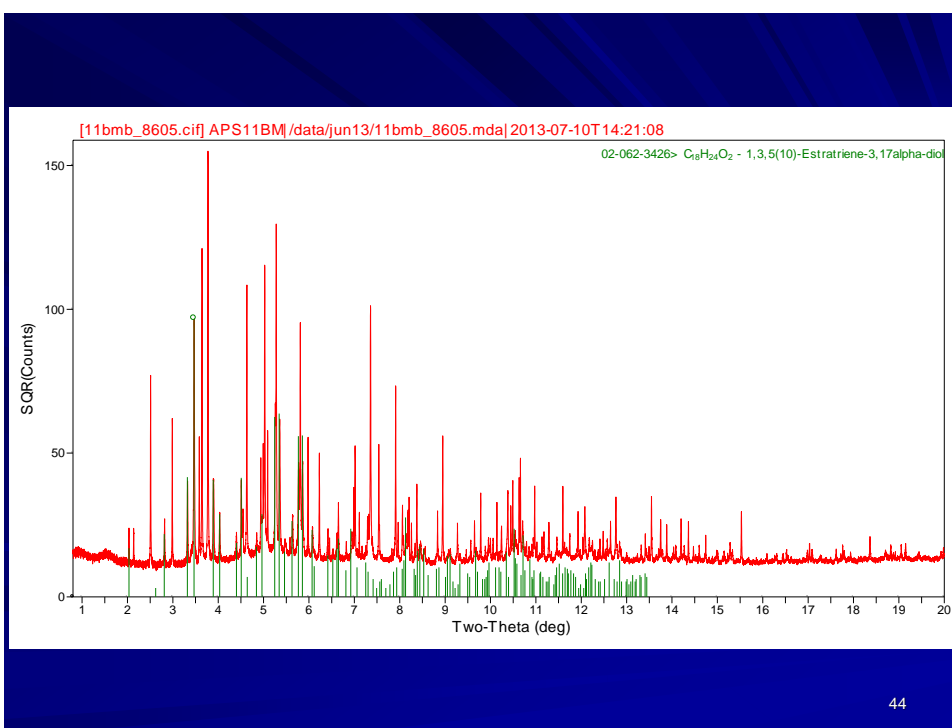
for treating hair loss in men and women

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## 17 $\alpha$ -Estradiol

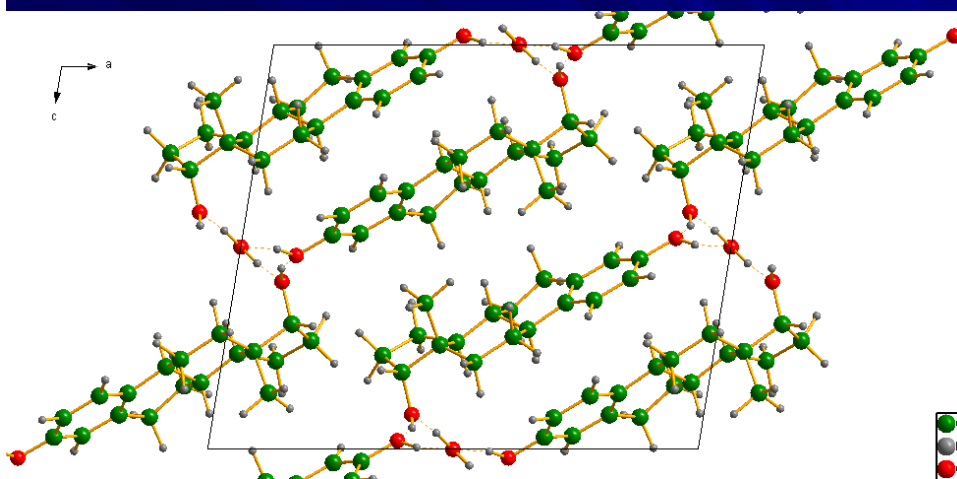


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## *beta 17 $\alpha$ -estradiol hemihydrate*



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*There is wonder in everyday materials!*



*Powder diffraction can yield new and interesting information about virtually everything we encounter everyday.*

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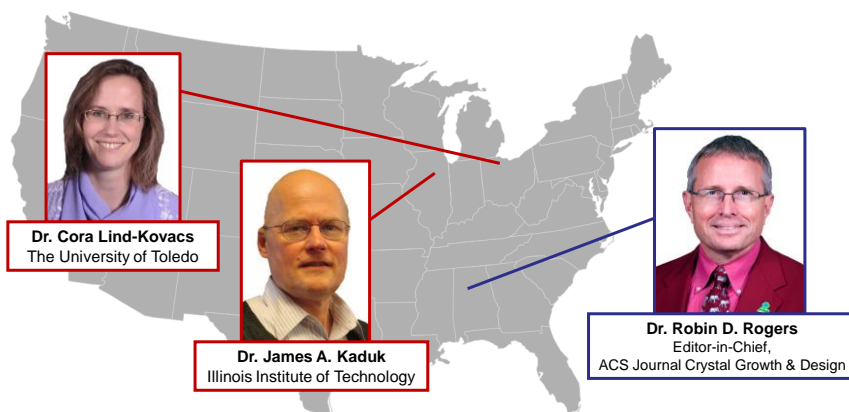
Question Slide: Do you think that crystallography ever made a positive impact on your work?

- Yes
- No
- Not sure

## ***Crystallography Resource Slide***

- 2014 is the International Year of Crystallography!
  - [iycr2014.org/](http://iycr2014.org/) (history, media resources, hands-on activities, competitions, schools & short courses, conferences...)
- International Union for Crystallography, [www.iucr.org](http://www.iucr.org)
- American Crystallographic Association, [www.americalcrystallography.org/](http://www.americalcrystallography.org/)
- International Centre for Diffraction Data, [www.icdd.com](http://www.icdd.com)
- Argonne National Lab Crystallography Education resources
  - [www.aps.anl.gov/Science/Courses/](http://www.aps.anl.gov/Science/Courses/)
- [en.wikipedia.org/wiki/X-ray\\_crystallography](http://en.wikipedia.org/wiki/X-ray_crystallography)

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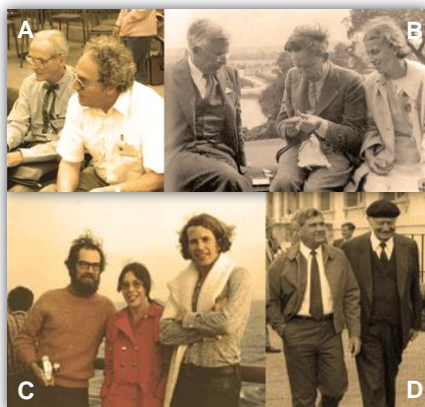


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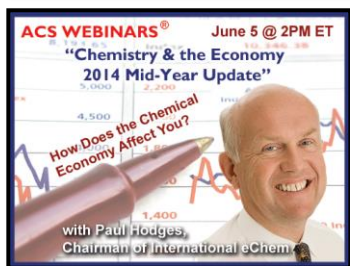
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Paul Hodges, Chairman of International eChem (leC)

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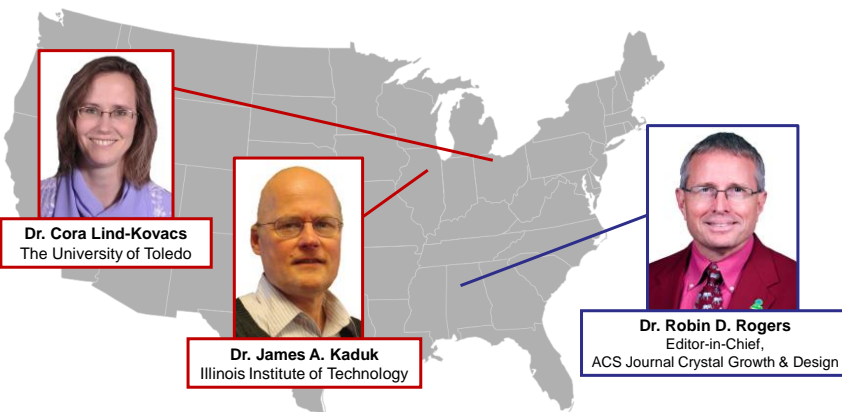
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Joshua Zars, MBA, MS, BS, BA,  
Regional Marketing Manager  
Baking Enzymes,  
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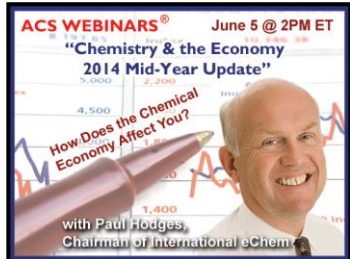
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