We will start momentarily at 2pm ET

Slides available now! Recordings will be available to ACS members after two weeks
 http://acswebinars.org/crystallography

Contact ACS Webinars ® at acswebinars@acs.org

Have Questions?

“Why am I muted?”
Don’t worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

Type them into questions box!

Contact ACS Webinars ® at acswebinars@acs.org
Have you discovered the missing element?

www.join.acs.org

Find the many benefits of ACS membership!

Like us on Facebook!

facebook.com/acswebinars
How has ACS Webinars® benefited you?

“allows me to take time each week and reconnect with my passion for Chemistry now that I am more involved with the business side of things at my job.”

Fan of the Week
Joshua Zars, MBA, MS, BS, BA,
Regional Marketing Manager
Baking Enzymes,
DSM Food Specialties USA, Inc.

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

Co-produced with the American Crystallographic Association

ACA History through photos!
A) William Lipscomb and Herbert Hauptman at an IUCr Congress and General Assembly.
B) Irving Langmuir, J.D. Bernal and Dorothy Hodgkin at the 1937 British Association Meeting.
C) Walter Hamilton, Helen Berman, and Tom Koetzle on their way to a meeting in Aarhus in 1972.

http://www.amercrystalassn.org
Missed last year’s webinar on Fulbright Core and Specialist Programs? Applications for these programs are coming due again this August 2014. Speakers from the Council for International Exchange of Scholars will join us again to give listeners an introduction to the various opportunities within the Fulbright Scholars Program for sending American scholars abroad and bringing scholars from overseas to the United States.
Hungry for a brain snack?

“ACS Webinets™ are 2 minute segments that bring you valuable insight from some of our most popular full length ACS Webinars®.”

See all the ACS Webinets at youtube.com/acswебinars

Beginning in 2014 all recordings of ACS Webinars will be available to current ACS members two weeks after the Live broadcast date.

Live weekly ACS Webinars will continue to be available to the general public.

Contact ACS Webinars® at acswебinars@acs.org
Celebrate 2014, International Year of Crystallography!

http://www.iycr2014.org/
ACA History through photos!

A) William Lipscomb and Herbert Hauptman at an IUCr Congress and General Assembly.

B) Irving Langmuir, J.D. Bernal and Dorothy Hodgkin at the 1937 British Association Meeting.

C) Walter Hamilton, Helen Berman, and Tom Koetzle on their way to a meeting in Aarhus in 1972.


http://www.amercrystalassn.org

Upcoming ACS Webinars®
www.acs.org/acswebinars

Thursday, May 29, 2014

Drug Discovery Series - Session 4
“Lead Optimization – Building Efficacy & Safety”

Dr. Craig Lindsley, Vanderbilt University
Dr. Joseph Fortunak, Howard University

Thursday, June 5, 2014

“Chemistry & the Economy: 2014 Mid-Year Update”

Paul Hodges, Chairman of International eChem (IeC)
Mark Jones, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org
“Crystallography Frontiers: How Chemistry Reveals the Wonder of Everyday Materials”

Slides available now! Recordings will be available to ACS members after two weeks
http://acswebinars.org/crystallography

This ACS Webinar is co-produced with the American Crystallographic Association

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
**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!

---

**Elemental Composition Is Not Enough**

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

---

*Structure Matters!*
Determining the 3D Structure of Solids

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

\[ 2d \sin(\theta) = n \lambda \]

First Crystal Structures

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

“This statement is more than repugnant to common sense it is absurd to the n\textsuperscript{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

Things we Take for Granted
Concepts Illuminated By Crystallography

- 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
Things we Take for Granted
Concepts Illuminated By Crystallography

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

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!
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

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!

http://www.periodictable.ru/050Sn/Sn_en.html
Understanding Everyday Materials using X-ray Powder Diffraction

James A. Kaduk
Illinois Institute of Technology
Chicago IL 60616
kaduk@polycrystallography.com

X-ray Diffraction

Single Crystal	Powder
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?
Table 1: Comparison of ingredients and contents of various peanut butter brands.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Ingredients</th>
<th>Skippy Creamy</th>
<th>Skippy Reduced Fat</th>
<th>Jif Reduced Fat</th>
<th>Smucker's Natural</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ingredients</td>
<td>peanuts</td>
<td>corn syrup sol.</td>
<td>peanuts</td>
<td>peanuts</td>
<td>peanuts</td>
</tr>
<tr>
<td></td>
<td>sugar</td>
<td>sugar</td>
<td>soy protein</td>
<td>corn syrup sol.</td>
<td>salt</td>
</tr>
<tr>
<td></td>
<td>salt</td>
<td>salt</td>
<td>salt</td>
<td>soy protein</td>
<td>hydr. veg. oils</td>
</tr>
<tr>
<td></td>
<td>hydr. veg. oils</td>
<td>mono/diglyc.</td>
<td>minerals</td>
<td>hydr. veg. oils</td>
<td>vitamins</td>
</tr>
<tr>
<td></td>
<td>sucrose, C₁₂H₂₂O₁₁</td>
<td>9.4</td>
<td>10.0</td>
<td>12.2</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>wt%</td>
<td>9.4</td>
<td>11.4</td>
<td>11.1</td>
<td>3.1</td>
</tr>
<tr>
<td>NI sugars, wt%</td>
<td>~1</td>
<td>~2?</td>
<td>~1</td>
<td>Small</td>
<td></td>
</tr>
<tr>
<td>Halite, NaCl</td>
<td>1.2</td>
<td>1.2</td>
<td>1.6</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>NI NaCl, wt%</td>
<td>-</td>
<td>0.2</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Dolomite, CaMg(CO₃)₂</td>
<td>-</td>
<td>1.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>β₂ fat, SSS</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Fat Molecule Structure

Determined in studies of chocolate!

Structure / Property Correlations

Propane Ammoxidation Catalysts
M1, TeNb(V,Mo)$_3$Mo$_6$O$_{30-x}$
US Patent 8,697,596 (Ineos USA LLC)

Claims on:
- Unit cell volume ~2250-2350 Å³
- Aspect ratio ~0.7-2.0
- Composition ranges

“Every catalyst I have ever studied at/near reaction conditions has had a different structure than at ambient!”
Thermal Expansion in 21207-66-48 GL#2 2-18-08

Temperature, °C

Relative Cell Volume

- major phase, vacuum
- minor phase, vacuum
- major phase, air
- minor phase, air

Commercial Pharmaceuticals

17α-Estradiol
Ell-Cranel Alpha, Pantosin
for treating hair loss in men and women
17α-Estradiol

![Chemical Structure of 17α-Estradiol]

![Graph of Two-Theta vs. SQR(Counts)]
There is wonder in everyday materials!

Powder diffraction can yield new and interesting information about virtually everything we encounter everyday.
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/ (history, media resources, hands-on activities, competitions, schools & short courses, conferences…)

- International Union for Crystallography, www.iucr.org
- American Crystallographic Association, www.amercrystalassn.org/
- International Centre for Diffraction Data, www.icdd.com
- Argonne National Lab Crystallography Education resources
  - www.aps.anl.gov/Science/Courses/
  - en.wikipedia.org/wiki/X-ray_crystallography
“Crystallography Frontiers:
How Chemistry Reveals the Wonder of Everyday Materials”

Slides available now! Recordings will be available to ACS members after two weeks
http://acswebinars.org/crystallography

This ACS Webinar is co-produced with the American Crystallographic Association

Co-produced with the American Crystallographic Association

ACA History through photos!
A) William Lipscomb and Herbert Hauptman at an IUCr Congress and General Assembly.
B) Irving Langmuir, J.D. Bernal and Dorothy Hodgkin at the 1937 British Association Meeting.
C) Walter Hamilton, Helen Berman, and Tom Koetzle on their way to a meeting in Aarhus in 1972.

http://www.amer水晶assn.org
Upcoming ACS Webinars®
www.acs.org/acswebinars

Thursday, May 29, 2014
Drug Discovery Series - Session 4
“Lead Optimization – Building Efficacy & Safety”
Dr. Craig Lindsley, Vanderbilt University
Dr. Joseph Fortunak, Howard University

Thursday, June 5, 2014
“Chemistry & the Economy: 2014 Mid-Year Update”
Paul Hodges, Chairman of International eChem (IeC)
Mark Jones, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org

ACS Webinars®
“Crystallography Frontiers: How Chemistry Reveals the Wonder of Everyday Materials”

Dr. Cora Lind-Kovacs
The University of Toledo

Dr. James A. Kaduk
Illinois Institute of Technology

Dr. Robin D. Rogers
Editor-in-Chief, ACS Journal Crystal Growth & Design

Slides available now! Recordings will be available to ACS members after two weeks
http://acswebinars.org/crystallography

This ACS Webinar is co-produced with the American Crystallographic Association
How has ACS Webinars® benefited you?

“allows me to take time each week and reconnect with my passion for Chemistry now that I am more involved with the business side of things at my job.”

Fan of the Week
Joshua Zars, MBA, MS, BS, BA, Regional Marketing Manager Baking Enzymes, DSM Food Specialties USA, Inc.

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org
Fulbright Opportunities in 2015-16
May 15, 2014; 3:00pm EDT

www.acs.org/ic_fulbright2015
Missed last year's webinar on Fulbright Core and Specialist Programs? Applications for these programs are coming due again this August 2014. Speakers from the Council for International Exchange of Scholars will join us again to give listeners an introduction to the various opportunities within the Fulbright Scholars Program for sending American scholars abroad and bringing scholars from overseas to the United States.

ACS Webinars®
Top 3 benefits of ACS Membership

1. The ACS Career Navigator
Your home for leadership development, in-person and online professional education, market intelligence, and career services.

2. Chemical & Engineering News (C&EN)
Serving the Chemical, Life Sciences & Laboratory Worlds, C&EN is the preeminent weekly news source for chemists.

3. ACS Webinars Archive
Can’t attend the Live broadcasts? Get access to over 125 recordings and counting with every new ACS Webinar and watch at your convenience.

Discover the full list of benefits! www.join.acs.org
ACS Webinars® does not endorse any products or services. The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the American Chemical Society.

Contact ACS Webinars® at acswebinars@acs.org

Upcoming ACS Webinars®
www.acs.org/acswebinars

Thursday, May 29, 2014

**Drug Discovery Series - Session 4**
“Lead Optimization – Building Efficacy & Safety”

*Dr. Craig Lindsley*, Vanderbilt University

*Dr. Joseph Fortunak*, Howard University

Thursday, June 5, 2014

“Chemistry & the Economy: 2014 Mid-Year Update”

*Paul Hodges*, Chairman of International eChem (IeC)

*Mark Jones*, Executive External Strategy and Communications Fellow, Dow Chemical

Contact ACS Webinars® at acswebinars@acs.org