<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Welcome letter</td>
<td>p. 3</td>
</tr>
<tr>
<td>Previous meetings</td>
<td>p. 4</td>
</tr>
<tr>
<td>Sponsors</td>
<td>p. 5</td>
</tr>
<tr>
<td>Scientific program</td>
<td>p. 6</td>
</tr>
<tr>
<td>Abstracts</td>
<td>p. 8</td>
</tr>
<tr>
<td>Attendees</td>
<td>p. 33</td>
</tr>
</tbody>
</table>
Welcome to MOSSCS XXVII

We are very excited that you will be joining us for the 27th Midwest Organic Solid State Chemistry Symposium, which was inaugurated in 1988 as the retirement symposium for Prof. David Y. Curtin of the University of Illinois at Urbana-Champaign. During the previous 20 years, Curtin’s seminal work with Iain Paul helped to establish solid-state organic chemistry as a distinct discipline in the United States. That first meeting attracted a number of internationally renowned scholars who had gathered to honor David Curtin’s contributions to the field. One of the organizers of the Curtin Symposium, the late Peggy Etter, decided that this meeting could serve as an ideal forum for young scientists to share their work in an informal and supportive environment.

Since 1989, MOSSCS has met every year except one, and it has more than lived up to Peggy Etter’s original goal of expanding and diversifying the field of solid-state organic chemistry in the United States. Over the years, graduate students, postdocs, and undergraduates have given close to 600 lectures, often their first to an “outside” audience. Many of the current leaders in the field gave their first talk at a MOSSCS meeting, and several have returned the favor by hosting the conference themselves.

This year, in addition to the student speakers, we are delighted to have plenary lectures that will be delivered by Amy Sarjeant (Cambridge Crystallographic Data Centre), Matthew Peterson (Biogen), Christopher Bardeen (University of California at Riverside) and Tendai Gadzikwa (Kansas State University). And, as a first for this conference, Amy Sarjeant will lead a hands-on workshop on the use of the Cambridge Structural Database.

We hope that all of the talks will stimulate you to think more broadly about your own research, and that the meeting will be an opportunity to make new friends and renew old acquaintances.

Mark Hollingsworth

Christer Aakeröy
# Past MOSSCS Meetings

<table>
<thead>
<tr>
<th>Year</th>
<th>Location</th>
<th>Organizers</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOSSCS I</td>
<td>1988 University of Illinois</td>
<td>Ian Paul/Peggy Etter/Steve Byrn</td>
</tr>
<tr>
<td>MOSSCS II</td>
<td>1989 University of Minnesota</td>
<td>Peggy Etter/Joel Bernstein</td>
</tr>
<tr>
<td>MOSSCS III</td>
<td>1990 Purdue University</td>
<td>Steve Byrn</td>
</tr>
<tr>
<td>MOSSCS IV</td>
<td>1992 University of Nebraska</td>
<td>Craig Eckhardt</td>
</tr>
<tr>
<td>MOSSCS V</td>
<td>1993 Purdue University</td>
<td>Bart Kahr</td>
</tr>
<tr>
<td>MOSSCS VI</td>
<td>1994 University of Minnesota</td>
<td>Mike Ward</td>
</tr>
<tr>
<td>MOSSCS VII</td>
<td>1995 Indiana University</td>
<td>Mark Hollingsworth</td>
</tr>
<tr>
<td>MOSSCS VIII</td>
<td>1996 University of Nebraska</td>
<td>Craig Eckhardt</td>
</tr>
<tr>
<td>MOSSCS IX</td>
<td>1998 Kansas State University</td>
<td>Christer Aakeröy</td>
</tr>
<tr>
<td>MOSSCS X</td>
<td>1999 Eli Lilly</td>
<td>Susan M. Reutzel</td>
</tr>
<tr>
<td>MOSSCS XI</td>
<td>2000 Purdue University</td>
<td>Ken Morris/Steve Byrn</td>
</tr>
<tr>
<td>MOSSCS XII</td>
<td>2001 University of Nebraska</td>
<td>Craig Eckhardt</td>
</tr>
<tr>
<td>MOSSCS XIII</td>
<td>2002 University of Iowa</td>
<td>Leonard MacGillivray</td>
</tr>
<tr>
<td>MOSSCS XIV</td>
<td>2003 University of Minnesota</td>
<td>Mike Ward</td>
</tr>
<tr>
<td>MOSSCS XV</td>
<td>2004 Southern Illinois University</td>
<td>Lori Vermeulen</td>
</tr>
<tr>
<td>MOSSCS XVI</td>
<td>2005 Purdue University</td>
<td>Steve Byrn/Ken Morris</td>
</tr>
<tr>
<td>MOSSCS XVII</td>
<td>2006 University of Iowa</td>
<td>Leonard MacGillivray</td>
</tr>
<tr>
<td>MOSSCS XVIII</td>
<td>2007 University of Kentucky</td>
<td>Tonglei Li/Carol Brock</td>
</tr>
<tr>
<td>MOSSCS XIX</td>
<td>2008 Kansas State University</td>
<td>Christer Aakeröy/Mark Hollingsworth</td>
</tr>
<tr>
<td>MOSSCS XX</td>
<td>2009 University of Missouri St. Louis</td>
<td>Alicia Beatty</td>
</tr>
<tr>
<td>MOSSCS XXI</td>
<td>2011 Eastern Illinois University</td>
<td>Kraig Wheeler/Radu Semeniuc</td>
</tr>
<tr>
<td>MOSSCS XXII</td>
<td>2012 Missouri State University</td>
<td>Eric Bosch</td>
</tr>
<tr>
<td>MOSSCS XXIII</td>
<td>2013 University of Kentucky</td>
<td>Eric Munson</td>
</tr>
<tr>
<td>MOSSCS XXIV</td>
<td>2014 University of Iowa</td>
<td>Leonard MacGillivray/Lewis Stevens</td>
</tr>
<tr>
<td>MOSSCS XXV</td>
<td>2015 Purdue University</td>
<td>Tonglei Li/Steve Byrn</td>
</tr>
<tr>
<td>MOSSCS XXVI</td>
<td>2016 University of North Dakota</td>
<td>Qianli &quot;Rick&quot; Chu</td>
</tr>
</tbody>
</table>
Thank you to our sponsors!

Boehringer Ingelheim is one of the world’s 20 leading pharmaceutical companies. Since its founding in 1885, the family-owned company has been committed to researching, developing, manufacturing and marketing novel treatments for human and veterinary medicine.

CrystEngComm is the journal for innovative research covering all aspects of crystal engineering - the design, including synthesis of crystals and crystal growth, synthesis and evaluation of solid-state materials with desired properties.

The aim of Crystal Growth & Design is to stimulate cross fertilization of knowledge among scientists and engineers working in the fields of crystal growth, crystal engineering, and the industrial application of crystalline materials.

Bruker is one of the world's leading analytical instrumentation companies, Bruker systems cover a broad spectrum of applications in all fields of research and development and are used in all industrial production processes for the purpose of ensuring quality and process reliability.
XXVII Midwest Organic Solid State Chemistry Symposium (MOSSCS)
June 9-10, 2017
Kansas State University, Manhattan, Kansas

Friday, June 9 (Tadtman Boardroom, Alumni Center)

8:00 a.m. - 8:30 a.m.  Registration and Continental Breakfast

8:30 a.m. - 8:40 a.m.  Welcome to Symposium and Opening Remarks

8:40 a.m. - 10:20 a.m.  Scientific Session I (Christer Aakeröy, presiding)

  8:40 a.m. - 9:20 a.m.  K.1  Dr. Amy Sarjeant, CCDC, ACA President
  9:20 a.m. - 9:40 a.m.  T.1  Chamara A. Gunawardana, Kansas State University
  9:40 a.m. - 10:00 a.m.  T.2  Gonzalo Campillo-Alvarado, University of Iowa
  10:00 a.m. - 10:20 a.m.  T.3  Rachel Roccanova, University of Oklahoma

10:20 a.m. - 10:40 a.m.  Coffee break

10:40 a.m. - 12:00 p.m.  Scientific Session II (Jesús Valdez-Martínez, presiding)

  10:40 a.m. - 11:00 a.m.  T.4  Janaka Gamekkanda, Kansas State University
  11:00 a.m. - 11:20 a.m.  T.5  Shalisa Oburn, University of Iowa
  11:20 a.m. - 11:40 a.m.  T.6  Nandini Sarkar, Kansas State University
  11:40 a.m. - 12:00 p.m.  T.7  Adam Lechner, Kansas State University

12:00 p.m. - 1:00 p.m.  Lunch (provided)

1:00 p.m. - 3:00 p.m.  CCDC/CSD Workshop (led by Dr. Amy Sarjeant)

3:00 p.m. - 3:20 p.m.  Coffee break

3:20 p.m. - 5:00 p.m.  Scientific Session III (Bayram Saparov, presiding)

  3:20 p.m. - 3:40 p.m.  T.8  Bhupinder Sandhu, Kansas State University
  3:40 p.m. - 4:00 p.m.  T.9  Quintin Elliot, University of North Dakota
  4:00 p.m. - 4:20 p.m.  T.10  Kamal K. Ray, University of Iowa
  4:20 p.m. - 5:00 p.m.  K.2  Prof. Christopher Bardeen, UC Riverside

6:30 p.m. - 8:30 p.m.  Conference dinner (Tadtman Boardroom)
Saturday, June 10 (209 King Hall, Department of Chemistry)

7:50 a.m. - 8:20 a.m. Continental Breakfast (provided in the foyer of the Chemistry/Biochemistry Building, adjacent to King Hall)

8:20 a.m. - 10:00 a.m. Scientific Session IV

8:20 a.m. - 9:00 a.m. K.3 Dr. Matt Peterson, Biogen
9:00 a.m. - 9:20 a.m. T.11 Weiwei Tang, Purdue University
9:20 a.m. - 9:40 a.m. T.12 Manomi Perera, Kansas State University
9:40 a.m. - 10:00 a.m. T.13 Dylan Shields, University of Cincinnati

10:00 a.m. - 10:20 a.m. Coffee break

10:20 a.m. - 12:00 p.m. Scientific Session V

10:20 a.m. - 10:40 a.m. T.14 Shane Nichols, New York University
10:40 a.m. - 11:00 a.m. T.15 Bo Wang, Kansas State University
11:00 a.m. - 11:20 a.m. T.16 Micah Mabin, University of North Dakota
11:20 a.m. - 11:40 a.m. T.17 Yue Qiu, University of Wisconsin-Madison
11:40 a.m. - 12:00 p.m. T.18 Stefan Andree, Kansas State University

12:00 p.m. - 1:00 p.m. Lunch (provided in the foyer of ChemBiochem)

1:10 p.m. - 2:50 p.m. Scientific Session VI

1:00 p.m. - 1:20 p.m. T.19 Zijun D. Wang, University of North Dakota
1:20 p.m. - 1:40 p.m. T.20 Shweta P. Yelgaonkar, University of Iowa
1:40 p.m. - 2:00 p.m. T.21 Prof. Jesus Valdés-Martínez, UNAM, Mexico City
2:00 p.m. - 2:30 p.m. K.4 Prof. Tendai Gadzikwa, Kansas State University
2:30 p.m. -2:50 p.m. Presentation of awards and closing remarks
K1. Understanding the solid form pharmaceutical landscape – 893,149 structures at a time.

Amy A. Sarjeant,¹ Shyam Vyas,¹ Neil Feeder,²...
¹The Cambridge Crystallographic Data Centre, Piscataway NJ, USA
²The Cambridge Crystallographic Data Centre, Cambridge UK

E-mail: sarjeant@ccdc.cam.ac.uk

The Cambridge Structural Database (CSD) now contains over 890,000 entries describing a vast array of crystal structures, from small drug-like compounds to massive metal—organic frameworks. While individual structures are informative in their own right, it is the knowledge gained from the entire collection together that powers scientific innovation. The structural information derived from the entries in the CSD can be used to answer questions concerning the stability, solubility, and solid form landscape of pharmaceutical compounds. This talk will feature several short stories of research successes and failures in the realm of pharmaceutical drug design and development, describing how an understanding of solid state chemistry and structural informatics can improve the success rates for creating new medicines.

Figure 1: The Full Interaction Map for a sulfathiazole target molecule.
K2. Turning photons into mechanical motion using molecular crystals

Christopher J. Bardeen

Department of Chemistry, University of California, Riverside, Riverside, CA 92521

E-mail: christob@ucr.edu

Molecular crystals allow one to organize photochemically reactive molecules and coordinate molecular motions so they give rise to microscale or macroscale deformations under light exposure.[1] Thus these materials provide one pathway to photomechanical actuators that can be scaled down to micro- or nanoscale dimensions. Anthracene derivatives that can undergo [4+4] photodimerization or cis-trans photoisomerization reactions provide a robust platform to make crystals that show strong photomechanical response. By modifying the molecular structure, it is possible to control the rate and reversibility of the solid-state photochemical reaction.[2] By tuning growth conditions, it is possible to generate crystals with a variety of shapes and sizes. For example, branched microcrystals of 4-fluoroanthracene carboxylic acid (4F-9AC) can be made using controlled solvent growth.[3] These microcrystals show twisting of the branches under illumination, which drives a rotation of the overall crystal that can be repeated over many exposures to light, thereby leading to ratchet-like motion.[4] Other types of photomechanical molecular crystals can undergo a variety of light-induced motions, including expansion, bending, twisting, curling and coiling. To quantitatively analyze the solid-state reaction kinetics and crystal motions, we have recently developed an extended Finke-Watzky model and derived rigorous equations to describe the photomechanical kinetics in solid-state molecular crystals of 9-methylnanthracene.[5] This analysis will help provide a systematic framework for understanding how chemical reaction dynamics produce largescale motions.

References


Pharmaceutical Sciences at Biogen involves several disciplines working together to advance compounds from research into development. For most compounds efficiency is emphasized over thoroughness. However, for compounds that advance into clinical development thoroughness is emphasized. Solid state chemistry influences many of the decisions made during this part of development. This presentation will highlight some of the Preformulation, Process Analytical, Material Characterization, and Biopharmaceutics activities and challenges associated with a development compound. The activities span chemical reaction monitoring, crystal form identification and characterization, characterization of material properties, and development of in silico and in vitro indicators of in vivo performance, with a common goal of developing robust and reliable products and manufacturing processes.

Figure 1: Packing diagram showing space occupied by solvent and voids left when solvent is removed (top), and photomicrographs showing crystal collapse as desolvation occurs (bottom).
K4. Multifunctional metal-organic framework materials for uniformly multivariate crystals

Tendai Gadzikwa, Christopher Satterfield, Kanchana Samarakoon, Mechelle McCoy

Kansas State University, Manhattan, KS, USA

E-mail: gadzikwa@ksu.edu

Metal-organic frameworks (MOFs) are microporous, crystalline materials, which have found application in the areas of separation, sequestration, detection, and catalysis, among many others. One of the main draws of MOFs is that, while having many favorable properties of solid state materials, these materials can also undergo organic transformations much like small molecules in the solution phase. Via the process of post-synthesis modification (PSM), chemists are able to decorate the internal surfaces of these materials with whichever functional groups are most useful for a given application.\(^1\) Within the class of modified MOFs is a subset in which the frameworks are elaborated with two or more organic modifiers, resulting in cavities bearing multiple functional groups.\(^2\) These so-called multivariate MOFs are attractive for applications involving cooperative interactions within a single cavity, with the most notable application being enzyme mimetic catalysis.

Current examples of multivariate MOFs are ones in which the multiple functionalities are inhomogeneously dispersed throughout the framework, meaning that the cavities of the material have non-uniform behaviors and properties. While this non-uniformity is of no adverse consequence in some applications, in catalysis it leads to poor selectivity.\(^3\) This talk will present efforts towards synthesizing uniformly, multivariate MOF frameworks, via a orthogonal post-synthetic modification strategy.

References

T1. Diamondoid networks from halogen-bonded halides

Chamara A. Gunawardana,1 Marijana Đaković,2 Abhijeet S. Sinha1 and Christer B. Aakeröy1

1Department of Chemistry, Kansas State University, Manhattan, Kansas 66506, United States.
2Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia.

E-mail: chamara@ksu.edu

We synthesized tetra(4-iodoethynyl)-substituted tetraphenylmethane [i.e. tetrakis(4-iodoethynyl)phenyl)methane, \( \text{I}_4\text{TPM} \)] with the intension of constructing 3-D supramolecular architectures by using the iodoethynyl functionality as a halogen-bond (XB) donor. \( \text{I}_4\text{TPM} \) was then subjected to a series of co-crystallization experiments, and it was found that this tetrahedral building block readily forms crystalline solids with tetraphenylphosphonium halides, \( \text{Ph}_4\text{P}^+\text{X}^- \) (\( \text{X}^- = \text{Cl}^-, \text{Br}^-, \text{I}^- \)).

The structural analysis revealed a 1:1 stoichiometry and diamond-like assembly wherein halide ions exhibit mutual-induced tetracoordination.[1] Moreover, in all these anionic frameworks, the function of tetraphenylphosphonium counterion seems to be two-fold; providing topological control/templating information and stabilizing the crystal lattice by residing in the void space.

Reference
T2. Boronic esters as supramolecular tools to form complex host-guest systems and direct solid-state reactivity


1 Department of Chemistry, University of Iowa, Iowa City, Iowa 52242, United States
2 Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, C.P. 62209 Cuernavaca, México

e-mail: gonzalo-campillo-alvarado@uiowa.edu

Organoboron compounds are among the most versatile and valuable intermediates in organic chemistry [1]. Boronic esters, a class of organoboron compounds resulting from the interaction of a boronic acid and a diol, have also attracted attention in the field of supramolecular chemistry owing to the ability to self-assemble into complex architectures via the N→B dative bonds with suitable Lewis bases [2,3]. In this context, boronic esters offer a broad window of opportunities to modulate and control the properties and reactivity of solids.

In this presentation, we will discuss the use of the N→B dative bond to generate boronic ester-based adducts with pyridyl-containing molecules. The adducts show the ability to include multiple guests in the crystal lattice facilitated by C−H···F and π···π interactions self-assembling into solvates and cocrystals. We will also discuss our preliminary efforts to direct reactivity of alkenes in the solid state using the N→B bond.

Figure 1: Crystal structure of a benzene molecule surrounded by four units of boronic ester-based adducts.

References
T3. Single crystal growth and characterization of R₂CdX₄ (R = CH₃NH₃, C₈H₅C₂H₄NH₃; X = Cl, Br, I) for scintillator applications

Rachel Roccanova,¹ Bayrammurad Saparov¹
²University of Oklahoma, Norman, USA

E-mail: rvow@ou.edu

Organic-inorganic hybrid materials have recently sparked the materials research community’s attention due to their excellent optoelectronic properties and their broadly tunable crystal structures and chemical compositions. The burgeoning field is most known for of the high efficiency photovoltaic material CH₃NH₃PbI₃ [1, 2, 3]. Through compositional and chemical changes, use of hybrid compounds can also be broadened to include scintillator materials for ionizing radiation detection, multiferroics, light-emitting diodes, photodetectors, etc [4, 5].

Here we present the results of our single crystal growth experiments for the organic-inorganic hybrid series (R)₂CdX₄ (R = CH₃NH₃, C₈H₅C₂H₄NH₃; X = Cl, Br, I) carried out by stoichiometric reactions in various solvent systems, producing single crystals of varying sizes. An optimized crystal growth condition yielded a 4 mm x 4 mm x 2 mm single crystal of (CH₃NH₃)₂CdCl₄. Single crystal and powder X-ray diffraction experiments suggest that the chloride analogs of (CH₃NH₃)₂CdCl₄ and (C₈H₅C₂H₄NH₃)₂CdCl₄ crystallize in 2D layered perovskite-derived structures based on corner-sharing CdCl₆ octahedra in space group Cmca with a = 7.384 Å, b = 19.220 Å, and c = 7.483 Å and Pbca with a = 10.8832 Å, b = 12.2191 Å, and c = 21.110 Å, respectively. In contrast, (R)₂CdBr₄ and (R)₂CdI₄ adopt 0D structures featuring isolated tetrahedral CdX₄ units separated by organic cations ((CH₃NH₃)₂CdBr₄: space group P2₁/c, cell parameters a = 8.122 Å, b = 13.4355 Å, and c = 11.4194 Å; (C₈H₅C₂H₄NH₃)₂CdBr₄: space group P2₁/c, cell parameters a = 7.8680 Å, b = 25.864 Å, and c = 11.0185 Å; (CH₃NH₃)₂CdI₄: space group Pbca, a = 10.9700 Å, b = 12.1576 Å, and c = 20.862 Å; (C₈H₅C₂H₄NH₃)₂CdI₄: space group P2₁, a = 10.940 Å, b = 8.214 Å, c = 13.556 Å). Simple room temperature synthesis and crystal growth [6, 7], and their band structures make R₂CdX₄ compounds promising candidates for scintillator applications.

Figure 1: (CH₃NH₃)₂CdX₄ structures determined from SXRD.

References
T4. Crystal engineering of energetic materials: Co-crystals of nitrocarbamates and nitriminotetrazoles with modified properties

Janaka Gamekkanda Gamaethige, Abhijeet S. Sinha and Christer B. Aakeröy

Kansas State University, Manhattan, KS, USA
E-mail: Janaka@ksu.edu

Explosives, propellants, and pyrotechnics are capable of delivering large amounts of energy very rapidly. Unfortunately, these substances are often very sensitivity to environmental conditions, such as heat, shock or friction which in turn, leads to considerable challenges when it comes to handling, storage, and transportation. Rather than making completely new explosive materials (which is very costly), and simply hoping that they will be more stable and safe to use, it is essential that we develop new technologies that are cost effective, scalable, easily implemented, and fast.

Co-crystallization is emerging as a new technology for modifying or enhancing the properties of energetic substances. In this process, the targeted energetic compound is combined with either an energetic material or a non-energetic material via non-covalent interactions. We are currently exploring this approach for improving the stability of a family of explosives that are inherently acidic and impact sensitive. (Scheme 1) Nitrocarbamates are known energetic materials which have acidic hydrogens that lead to compounds that are corrosive and unstable. Nitriminotetrazoles are recognized as explosive materials that are highly sensitive towards impact and they also possess relatively low decomposition temperatures. In order to stabilize and improve properties of these energetic materials, a co-crystallization approach has been utilized by introducing nitrogen or oxygen based hydrogen-bond acceptors.

![Scheme 1: Chemical structures of (a) pentaerythritol tetranitrocarbamate and (b) 2-methyl-5-nitriminotetrazole which can act as hydrogen-bond donors](image)

According to the results, we have found that the new co-crystals display different impact and thermal sensitivity as compared to the original explosives, and the corrosiveness has been dramatically reduced.

References
**T5. Functional groups as determinants in the engineering of mechanical properties of cocrystals**


Department of Chemistry, University of Iowa, Iowa City, IA, 52242
E-mail: Shalisa-oburn@uiowa.edu

Aims to achieve solid materials with well-defined physical and mechanical properties are a major focus in the field of supramolecular chemistry. Mechanical properties of crystalline materials are central in the pharmaceutical industry as they typically dictate the tabletability, milling, and compression properties of solids.[1] In this sense, overall molecular packing can give rise to drastic variation in bulk crystalline properties such as stiffness, granularity, dissolution rates, and strain sensitivity; although, inherent issues arise due to a lack of understanding of structure-property relationships.[2] We have recently reported a correlation between atomic polarizability of halogenated cocrystals and elasticity, with iodine as the most polarizable atom supporting the softest and most polarizable cocrystal.[3] Here we sought to investigate the relationship between functional group (i.e. alkene and alkane) and crystalline mechanical properties. Specifically, we compare the elasticity and polarizability of two isostructural cocrystals based on salicylic acid that contain a cocrystal former with either an alkene or alkane. Two polymorphs containing alkene functionalities are also assessed. We present structural attributes (e.g. functional groups, non-covalent interactions) that we attribute to give rise to variations in mechanical properties of specified cocrystals.

![Graph showing variations in elasticity and polarizability of salicylic acid cocrystals.](image)

**Figure 1: Variations in elasticity and polarizability of salicylic acid cocrystals.**

**References**

Cavitands are organic host molecules enforced with bowlshaped cavities which are capable of encapsulating cations, anions, solvents and guest molecules. There are various applications of cavitands and all these are characteristic of the defined space, volume and functional group of the host. The structural framework of a cavitand can be divided into four parts: feet, body, upper rim and bridge. Covalent modifications to the “feet” improves solubility, the “body” contains the p-cloud where electron deficient guest molecules are captured, the “upper rim” can be modified with different functional groups and the “bridges” determines the width of the cavitand.

In this study we focus our efforts mainly on covalent modifications to the “upper rim” of the cavitand. Resorcinarene-based cavitands were functionalized with groups such as bromo, iodo, carboxylic acid, trimethylsilyl, acetylene and pyridyl moieties. The most important applications of these cavitands arise due to the nature of the cavity. Several new functionalized cavitands were synthesized and the resulting solids were analyzed by IR and NMR spectroscopy, DSC and TGA and single crystal X-ray diffraction to further investigate the structural preferences of cavitands.

Figure 1: Structural framework of cavitand.

References
T7. Polymorphism in fumaronitrile and growth of cocrystals with urea

Adam Lechner, Bo Wang, Mark D. Hollingsworth
Kansas State University, Manhattan, KS

Email: adamlechner@ksu.edu

Prior studies have shown that layered complexes of 1:1 α,ω-dinitriles and urea exhibit a predictable hydrogen bonding motif that depends upon the chain lengths of their respective dinitriles [1,2]. Using this template, one can predict the hydrogen-bonding network as well as crystal morphology for α,ω-dinitriles of varying chain lengths – in this particular case, fumaronitrile ((2E)-2-Butenedinitrile) and urea, which had not been previously characterized.

The crystal structure of fumaronitrile alone was determined in 1982 by Doyle Britton and W. B. Gleason of the University of Minnesota [3]. In comparing powder X-ray diffraction (PXRD) patterns from a sample of fumaronitrile, it was discovered that over time, the compound spontaneously converts into a new polymorph (I). It was then hypothesized that the structure determined in 1982 was of a metastable form (II).

It was later found that through a solution-mediated transformation at room temperature followed by analysis with PXRD that fumaronitrile of Form I could be converted to Form II. This finding refutes the hypothesis that Form II – studied by Britton and Gleason – was a metastable polymorph and shows that Form I is less stable at room temperature. Thermal analysis via differential scanning calorimetry (DSC) further strengthened the previous findings by revealing a solid-solid phase transition at approximately 35-40 °C upon heating or cooling between the two forms, which are enantiotropically related. This furthermore suggests that the materials previously considered Form I were likely a mixture of the two forms and that pure Form I had yet to be obtained.

Previous studies showed that a 1:1 mixture of fumaronitrile and urea subjected to intensive grinding in a dental amalgamator known as a Wig-L-Bug reliably produces cocrystals in powder form, but single cocrystals had not yet been grown. With the intention of seeding a fumaronitrile and urea solution to grow single crystals for X-ray diffraction, polycrystalline cocrystals of fumaronitrile and urea were prepared following the Wig-L-Bug procedure. This proved to be unnecessary, as a simple room temperature evaporation in methanol gave single crystals suitable for X-ray diffraction. Currently, the goal is to obtain an X-ray dataset of the newly grown single crystals and use it to solve the crystal structure of the 1:1 cocrystal of fumaronitrile:urea.

References
T8. Predicting hydrogen bonding in organic crystals using propensity model

Bhupinder Sandhu, a Dr. Christer B. Aakeröy, a Dr. Susan M. Reutzel-Edens, b Dr. Amy A. Sarjeant, c Dr. Shyam Vyas c

aDepartment of chemistry, Kansas State University, Manhattan, Kansas, USA
bLilly Research Laboratories, Eli Lilly and Co., Indianapolis, Indiana, USA
cThe Cambridge Crystallographic Data Centre, Piscataway, New Jersey, USA

E-mail: bhupindersandhu90@ksu.edu

Crystallization and polymorphism play an important role in the development and performance of a drug. [1] An enormous amount of effort goes into generating the first seed crystal, and determining various crystal forms usually by empirical screening approaches. Despite an extensive amount of research in this field, it is still difficult to predict, simply from the chemical structure, the number of crystal forms of a compound and how to control and prepare unknown crystal forms. The Cambridge Structural Database (CSD) has developed a knowledge-based model within the Mercury software which is based on the hydrogen-bond propensity of a molecule. [2] In our study, the model is tested on small, rigid molecules such as thiazole and pyrazole with multiple hydrogen bond donors and acceptors. The goal of the study is to determine whether hydrogen-bond propensity (for substituent’s at ortho, meta and para position) predicted by the model agrees with the experimentally obtained crystal structure. These results were supported by molecular electrostatic potentials, DSC and crystal structures of the ligands (scheme 1). The knowledge gained from this study will be applied to more flexible, larger drug-like molecules with higher complexity.

Scheme 1: Outline of our hydrogen bond propensity study

References
T9. Black lights serving as a mild, facile, and frugal irradiation source to synthesize a diacid building block

Quintin Elliott, Zijun Wang, Joseph Lee, Dr. Qianli R. Chu*
University of North Dakota, Grand Forks, Grand Forks County

E-mail: quintin.elliott@und.edu

Solid-State [2+2] photocycloaddition has been shown to be a method that can produce unique monomers and polymers. However, traditional irradiation methods, such as sunlight and mercury-arc lamp have. Sunlight can be an inconstant irradiation source as one’s longitudinal location, weather patterns, and broad irradiation wavelengths can make it challenging to provide a sample with proper irradiation. Mercury-arc lamps are a costly and harsh irradiation source that in addition to emitting a broad range of wavelengths require external and/or expensive equipment to operate.

Black lights provide one with a mild, facile, frugal, and reliable irradiation source for certain photoreactions. Black lights are a mild irradiation source that can run on ~15 watts/hour without the production of superfluous amounts of heat. As a result of using black lights as an irradiation source our research group has successfully managed to dimerize furanacrylic acid in high purities on a multigram scale reaction. This is a challenging reaction because a significant amount of impurity have been observed when preformed under sunlight irradiation. The reactions with black lights were able to be carried out either by directly using powder furanacrylic acid or by means of a slurry in a poor solvent such as hexane. The single crystal structure of the diacid product revealed the geometry of the molecule and orientation of the two dicarboxylic acid groups showing its potential to serve as a building block in materials.

References
T10. Modulation of electrical conductivity of π rich organic molecules’ guests in boronic ester adduct host

Kamal K. Ray,1 Gonzalo Campillo-Alvarado,1 Herbert Höpfl,2 Hugo Morales-Rojas,2 Leonard R. MacGillivray1 and Alexei V. Tivanski1

1Department of Chemistry, University of Iowa, Iowa City, Iowa 52242, United States
2Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, C.P. 62209 Cuernavaca, México

E-mail: kamalkanti-ray@uiowa.edu

Modulation of the supramolecular constructions of organic molecules and the control of the desired optical, electrical and mechanical properties of the molecules are the central aims of crystal engineering [1]. In particular, synthesis of successful organic semiconductors depends on the proper engineering strategies. In this context, aromatic organic compounds with π-π interactions and their relative molecular orientation in the crystal structure determines the efficiency of the charge transport through the organic semiconductors [2,3]. Recently, we have studied charge carrier mobility of semiconducting organic assemblies prepared from tetraphenylethylene tetracarboxylic acid and bis(pyridine)s via charge-assisted hydrogen bonding. [4] Herein, we employ host-guest chemistry involving boronic ester adducts of 4,4'-bipyridine (bpy) as hosts to determine the variation of electrical conductivity based on the modification of the guest. More specifically, study of charge carrier mobility of the π rich organic guests pyrene and tetrathiafulvalene (TTF) in the boronic-based host was performed on an individual nano-crystal basis using conducting probe atomic force microscopy. Our results show how mechanical and electrical properties change depending on the organic guest molecule. These distinctions can be partially attributed to the differences in the extended π stacking crystal structure within these solids.

Figure 1: Variation of current density of TTF (green) and pyrene guest (pink) in boronic ester adduct host

References
T11. Why is Glycine’s polymorphism pH-dependent? A perspective from self-association in solution

Weiwei Tang,1 Huaping Mo,2 Mingtao Zhang,1 Tonglei Li1,*

1Department of Industrial and Physical Pharmacy, 2Department of Medicinal Chemistry and Molecular Pharmacology, College of Pharmacy, Purdue University, West Lafayette, IN 47907

E-mail: tang248@purdue.edu/tonglei@purdue.edu

Glycine (Gly) is recurrently debated mainly regarding to its formation of hydrogen-bonded cyclic dimer in pure water and the explanation on selective nucleation of α form due to the presence of such dimer.1-4 Our recent study explores this interesting phenomenon from a different perspective and systematically investigates the self-association of Gly in D2O and H2O, as well as aqueous solution in a wide range of pH, through utilizing 1D and 2D NMR and FTIR spectroscopy, as well as density functional theory (DFT) calculation. The results show that glycine molecules do self-associate in both D2O and H2O with about the same dimerization constant forming chain-like dimer. The solution speciation of Gly was further explored in aqueous solutions at various pH values, and it was found that the appearance of Gly associates is significant in the pH domains 3-9 but drops rapidly from the two pH extremes. Consequently, the apparent connection between the appearance of solute associates and always nucleation and growth of α form in the pH range 3-9 (including in water) suggests the Gly zwitterion associates is a necessary condition but not sufficient for α form formation. On the other hand, we found the crystallization of γ form may be a cluster alignment-controlled process where the charged species (cation or anion at pH<3 or pH>9) helps the alignment of γ nuclei easing the nucleation barrier. The findings highlight the roles of pre-nucleation solution aggregates in determining the formation of organic crystalline polymorphs.

Figure 1: Top: The chemical shift variations of methylene protons at the two extreme Gly concentrations as a function of pH in aqueous solution. The chemical shift difference between the two concentrations indicates formation of Gly associates in solution. Bottom: The labeled bar presents the crystallization outcomes of Gly in aqueous solution.

References
T12. Halogen-bond based catalysis: An alternative to hydrogen-bond based catalysis

Manomi Perera¹, Christer B.Aakerøy¹
¹Department of Chemistry Kansas State University, Manhattan, KS 66506-0401, USA

E-mail: manomi@ksu.edu

Halogen bonds are considered to have fundamental similarities to hydrogen bonding and well studied in crystal engineering and self assembly processes. [1] There is a growing interest in halogen-bond based molecules in solution phase, as catalysts similar to well-known hydrogen-bond based organocatalysis. However, there are only few mutidentate halogen-bond donors reported and the synthesis and design is significantly challenging due to the limited availability of precursors. Therefore, to date halogen-bond based catalysis is still an emerging area and there are only few examples reported. [2-3] In this study we designed a multidentate halogen-bond donor molecule using an iodine atom as the donor moiety. Activation of the iodine group to form strong halogen bonds was carried out by activation through a sp hybridized carbon atom. To establish the potential for halogen-bond donors in catalysis, two control molecules, one without any halogen bond donor and one without activating the halogen bond donor was synthesized. Catalysts were applied to a benchmark Ritter type solvolysis of benzhydryl bromide reaction. Results were analyzed through 1H NMR spectroscopy. Our results suggest catalytic activity in the presence of the halogen-bond based donor molecule, whereas no activity was found in the control system.

Figure 1: Halogen bond based catalyst (a) and the control molecules (b and c)

References
T13. Dancing crystals: The gas release mechanism of diazide naphthoquinones and the corresponding crystal motions

Dylan Shields¹, Stefan Schramm², Jeanette Krause¹, Durga Karothu², Anna D. Gudmundsdottir¹

¹University of Cincinnati, Cincinnati, Ohio, USA
²New York University Abu Dhabi, Abu Dhabi, UAE

shielddj@mail.uc.edu

The ability of polymers to convert light and heat into mechanical motions have been long been sought by researchers hoping to turn these materials into sensors, molecular machines, and medical devices[1-3]. However, polymers are not the only materials capable of producing mechanical motions as single crystals have shown the ability to reshape, jump, bend, twist, creep, and explode when exposed to external stimuli such as light and heat[4]. Recently there has been an interest in the use of single crystal actuators due to their ease of structural modification, faster response times, and more refined methods of investigation, such as X-ray crystallography[5]. The focus of this presentation will be on the crystal motions of 2,3-diazido-1,4-naphthoquinone and derivatives of this compound powered by the nitrogen gas release during irradiation of the crystals. The motions of these crystals have been characterized primarily using recorded optical microscopy, SEM imaging, and correlation to X-ray crystallography structures. In addition to the crystal motions, a mechanism for this denitrogenation reaction has been proposed by analyzing this reaction using picosecond LFP systems and DFT calculations in tandem to identify key intermediates.

References:

T14. Modeling optically active crystals in transmission, reflection, and fluorescence
Shane Nichols, Alexander Martin, Melissa Tan, Emily Timothy, Bart Kahr

New York University, Department of Chemistry and Molecular Design Institute, New York, NY 10003

E-mail: shane.nichols@nyu.edu

Quantitative characterization of optical activity in anisotropic crystals has long proven arduous. Optical activity is a material property in which left- and right-circular polarizations of light experience different refractive indices along certain directions in a crystal. The dispersive and absorptive parts are called circular birefringence and circular dichroism, respectively. Since the discovery of circular birefringence of quartz in 1811 by François Arago, only tens of compounds have been completely and quantitatively characterized. Difficulties arise because optical activity is a substantially smaller effect than linear anisotropy; the latter complicates measurement.

We demonstrated a method to model the transmitted and reflected fields by reckoning the finite coherence of light in spectroscopic devices [1]. In essence, different outgoing beams generated by multiple internal reflections are summed incoherently. Our model permits reflection measurements where light is taken from both the front and back interface, from which both the tensor of optical activity, and the electric permittivity tensor can be recovered together.

Optical activity is also manifest in fluorescence measurements. While results are sparse in this area, there is much interest in “fluorescence detected circular dichroism” and “circularly polarized luminescence” and how these quantities can be obtained from a fluorescence Mueller matrix (FMM). More generally, what are the signatures of optical activity experienced by light at the excitation and emission wavelengths? Early considerations of liquids [2] suggested that the two aforementioned quantities could be obtained directly from the anti-diagonal elements of the FMM. Using a new conoscopic FMM imaging system, we measured the FMM of an optically active and anisotropic crystal containing a dye impurity. Inferred by the data, we developed a general model from a solution to Maxwell’s equations in which the current density vector is retained. We successfully modeled the data, shown in the figure below, and learned that interpreting a FMM is quite complicated; FMM elements are not trivially connected to optical activity experienced at the excitation or emission wavelengths, much like a transmission Mueller matrix.

Figure 1: FMM of dye sunset yellow in ethylenediammonium sulfate showing data (left) and model (right).

References
T15. **Self-compression in phase transitions of a urea inclusion compound**

**Bo Wang, Ilya Frantsuzov, Mark D. Hollingsworth**  
*Kansas State University, Manhattan, USA*

E-mail: wangbo@ksu.edu

Urea inclusion compounds (UICs) are classic examples of nanoporous, host:guest materials in which the linear channels of the honeycomb structure of the urea host can include various types of long-chain compounds (the guests). By using synchrotron X-ray radiation sources, a deeper understanding of these materials is made possible through detailed structural studies. In particular, this presentation describes a series of structural phase transitions that occur upon cooling two related UICs containing alkanedione guest molecules.

UICs may be classified as either commensurate or incommensurate structures, depending on whether the repeat lengths of the host ($c_h$) and guest ($c_g$) along the channel axis are related by a small whole number ratio. Crystals of 2,8-nonanedione/urea and 2,11-dodecanedione/urea, which are incommensurate structures at room temperature, undergo “lock-in” phase transitions below room temperature to generate commensurate structures in which the guest repeat lengths are elongated. Upon nucleation and growth of these elongated, commensurate phases, other molecules in the same channels are compressed to give successively shorter guest repeat lengths. Further lock-in phase transitions give a multitude of commensurate and incommensurate phases during cooling. The crystal structures of two of these commensurate phases have been determined using synchrotron sources, as shown in Figure 1. The “self-compression” observed in these 1-D crystals serves as a paradigm for understanding solid-state reactions in three-dimensional crystals.

![Figure 1: Crystal structure of 2,8-nonanedione/urea, top, and 2,11-dodecanedione/urea, bottom.](image-url)
A series of five sorbic amide monomers were synthesized using a nucleophilic substitution reaction between sorbic acid and five diamine linkers. This formed double-sided or so-called “gemini” monomers with a photoreactive 1,3-butadiene group on both ends connected by a saturated carbon chain in the middle. These sorbic amide monomers have two possible advantages over similar gemini monomers. Firstly, the conjugated diene system of sorbic acid can form polyladderanes upon photopolymerization, which are multiple adjacent cyclobutane rings, as opposed to the single cyclobutane ring formed by polymerization of monomers with single, unconjugated olefins. The other advantage is that amides, as opposed to esters, can form hydrogen bonds with each other, resulting in higher melting points and possibly stronger polymers. Indeed, the melting points of these sorbic amide monomers were much higher (190-250 degrees) than their ester counterparts (60-100 degrees). The monomers were characterized using $^1$H- and $^{13}$C-NMR, IR, and UV/vis spectroscopy, HRMS, TGA, and P-XRD.

An attempt was made to polymerize these five monomers by [2 + 2] cycloaddition in the solid state using mercury lamps. The reaction was monitored by IR spectroscopy. For one of the monomers, SAC-4, IR showed the disappearance of all C-C double bonds in under 24 hours, indicating a high probability that a polyladderane was formed. For two of the other monomers, SAC-2 and SAC-5, the double bonds disappeared in less than 72 hours.

Figure 1: proposed [2 + 2] photocycloaddition of SAC-4 forming polyladderanes. Hydrogen bonding between amide groups is also shown.
T17. **Photostability can be significantly modulated by molecular packing in glasses**

Yue Qiu,¹ Lucas Antony,² Juan de Pablo², Mark D. Ediger¹

¹ Department of Chemistry, University of Wisconsin–Madison, Madison, WI 53706, USA  
² Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, USA

E-mail: yqiu@chem.wisc.edu

Photochemically robust materials are desired for organic electronics¹. While previous work has demonstrated that molecular packing in organic crystals can strongly influence photochemical stability, efforts to tune photostability in amorphous materials have shown much smaller effects²,³. In this work, we show that physical vapor deposition can substantially improve the photostability of organic glasses⁴. Glasses made of two organic molecules that can undergo different reaction types were studied as model systems. In the first case, photoisomerization of disperse orange 37 (DO37), an azobenzene derivative, was studied in both vapor-deposited and liquid-cooled glasses. Photostability is assessed through changes in density and molecular orientation of glassy thin films during light irradiation. In the second case, photodegradation of indomethacin, a drug molecule, was studied by directly monitoring the mass loss induced by photo-decarboxylation during the irradiation. For both cases, we show that the rate of photoreaction varies as a function of the substrate temperature during the deposition, and photostability correlates with glass density. Coarse-grained molecular simulations, which mimic glass preparation and the photoisomerization reaction, also indicate that glasses with higher density have substantially increased photostability. These results show for the first time that photostability of glasses can be significantly modulated by molecular packing. They provide insight that may assist in the design of organic photovoltaics and light emission devices with longer lifetimes.

References

T18. Self-assembly of halogen bond derivatized Tröger’s bases for formation of molecular squares

Stefan N. L. Andrée,1 Christer B. Aakeröy,2 A.S. Sinha
1 Department of Chemistry, Kansas State University, Manhattan KS, USA
2 Department of Chemistry, Kansas State University, Manhattan KS, USA

E-mail: snlandree@ksu.edu

The V-shape and C2-symmetry of the chiral molecule Tröger’s base, Figure 1, possess many interesting features. It consists of a bicyclic aliphatic unit fused with two aromatic rings, which are nearly perpendicular rendering the base, a concave shape which provides a hydrophobic cavity. The methylene bridge of this uniquely shaped molecule precludes pyramidal inversion of the two nitrogen atoms, making them configurationally stable stereogenic centers.

In this study, two new derivatives of this molecule were synthesized with a sharp emphasis on the directionality of a much less explored intermolecular interaction; the halogen bond, with the purpose of determining whether it can induce the formation of molecular squares. The reason behind this supramolecular synthesis is mainly functional, where these assemblies contain cavities that are capable, in principle, of encapsulating, sensing, processing, or transporting useful molecules or atomic ions.

For this purpose, a carefully selected list of ditopic acceptors were used, which can target the most prominent binding sites the “iodoethynyl sites” on the Tröger’s base with a precise combination. Subsequently, the study also aimed at examining the molecular electrostatic potentials of the respective iodoethynyl Tröger’s base derivatives and ditopic acceptors as a way of rationalizing intermolecular binding preferences.

The 2,8-bis(trimethylsilyl)ethynyl]-functionalized Tröger’s base a precursor, was determined by X-ray crystal structure analysis. Melting point and IR analysis were done to confirm the formation of four new cocrystals that were obtained. Differential Scanning Calorimetry (DSC) studies will be followed by X-ray crystallography on the cocrystals obtained.

![Figure 1: Tröger’s base](image-url)
T19. A building block for ladder-like polymers

Zijun D. Wang, a Quintin Elliott, and Qianli R. Chu*
University of North Dakota, Grand Forks, USA

E-mail: zijun.wang@und.edu

Ladder-like polymers are believed to possess desirable mechanical strength because the polymer strands can tolerate a breaking point in each repeating unit without falling apart.¹-² Unlike numerous single-stranded polymers, only a few ladder-like polymers have been reported. Their strands are mostly either non-covalently bonded, conformationally rigid or thermally reversible.³-⁴ We report herein the preparation of a monomer for a potential flexible and thermally irreversible ladder-like polymer, which is also a novel polycyclobutane.⁵ The flexibility is inherited from the flexible long alkyl chains and the thermal stability is due to the actuality that the ring opening of cyclobutane moiety is thermally forbidden.

Cyclic molecules with alkene moiety have been designed and synthesized. Single crystal structures of both cis and trans isomers of the monomer were obtained by X-ray diffraction. The polymerization has been conducted in solution and the product was isolated by simply filtration. FT-IR, solid-state NMR, and transesterification experiment confirmed the formation of the ladder-like polymer while oligomers were detected by HRMS. The polymer was proved to be stable under sunlight and under 100 °C after 1 month. DSC, TGA and SEM have been applied to characterize the thermal property and the macrostructure of this polymer, respectively.

Figure 1: cis isomer (left) and trans isomer (right) of the monomer.

References

T20. A product of a Diels-Alder reaction as a template in a solid-state reaction

Shweta P. Yelgaonkar and Leonard R. MacGillivray*

Department of Chemistry, University of Iowa, Iowa City, IA 52242, USA

shwetapandharinath-yelgaonkar@uiowa.edu

The use of the principles of supramolecular chemistry is a reliable means to organize molecules and design structural outcomes of solid-state reactions. We have introduced supramolecular strategy that utilizes templates to pre-organize olefins into the prerequisite geometry for a [2+2] photodimerization in the solid state [1]. We reported template switching as a supramolecular strategy to overcome issues of crystal packing and to achieve quantitative conversion [2]. To date, we have routinely utilized the rigidity of aromatic rings in designing our organic templates.

Inspired by previously reported non-aromatic templates Rebek’s imide [3] and rctt-1,2, 3,4-cyclobutanetetracarboxylic acid [4], we sought to utilize a non-aromatic, rigid norbornene molecule as the backbone for a new template. Herein, we report the exo,exo-7-oxa-5-norbornene-2,3-dicarboxylic acid (DAT) as a novel template. The DAT template has an appropriate molecular geometry to exploit the strength and directionality of hydrogen bonds and enforce the alignment of two carbon-carbon double bonds (C=C) within a discrete complex for a reaction in the solid state.

Reference
T21. Study of intermolecular interactions through multifunctional ligands

J. Valdés-Martínez, E. Jaime-Adan, M. J. Hernández-Vergara, A. D. Sánchez-Pacheco

*Universidad Nacional Autónoma de México, Instituto de Química, Cd. Mx., México*

E-mail: jvaldes@iquimica.unam.mx

The understanding of intermolecular interactions: hydrogen bond, halogen bonds and the interactions between aromatic rings —usually called $\pi-\pi$ interactions— is fundamental in crystal engineering. We have designed ligands that can interact between them through different interactions without interfering with each other, allowing the competition between three different interactions, see Figure 1.

![Family of ligands](image)

These ligands are easy to modify and allow studies on:

- The influence of different halogen atoms
- The effect of the number of fluorine atoms and/or its position on the interaction between the aromatic rings and the directionality of the interaction.
- The presence of fluorine atoms in the halogenated aromatic ring, allows week C-H $\cdots$ F interactions.[1]
- The synthesis of co-crystals and the changes of the observed interactions compared with the free molecules.

We will present different results illustrating the above-mentioned points.

**References**

### Attendees

<table>
<thead>
<tr>
<th>Name</th>
<th>Email</th>
<th>Affiliation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Christer Aakeröy</td>
<td><a href="mailto:aakeroy@ksu.edu">aakeroy@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Amila Abeysekera</td>
<td><a href="mailto:abeysekeramila@ksu.edu">abeysekeramila@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Stefan Andree</td>
<td><a href="mailto:snlandree@ksu.edu">snlandree@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Chris Bardeen</td>
<td><a href="mailto:christob@ucr.edu">christob@ucr.edu</a></td>
<td>University of California at Riverside</td>
</tr>
<tr>
<td>Gonzalo Campillo-Alvarado</td>
<td><a href="mailto:gonzalo-campillo-alvarado@uiowa.edu">gonzalo-campillo-alvarado@uiowa.edu</a></td>
<td>University of Iowa</td>
</tr>
<tr>
<td>Craig Eckhardt</td>
<td><a href="mailto:ceckhardt1@unl.edu">ceckhardt1@unl.edu</a></td>
<td>University of Nebraska at Lincoln</td>
</tr>
<tr>
<td>Quintin Elliott</td>
<td><a href="mailto:quentin.elliott@und.edu">quentin.elliott@und.edu</a></td>
<td>University of North Dakota</td>
</tr>
<tr>
<td>Tendai Gadzikwa</td>
<td><a href="mailto:gadzikwa@ksu.edu">gadzikwa@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Janaka Gamekkanda Gamaethige</td>
<td><a href="mailto:janaka@ksu.edu">janaka@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Chamara Gunawardana</td>
<td><a href="mailto:chamara@ksu.edu">chamara@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Mark Hollingsworth</td>
<td><a href="mailto:mdholl@ksu.edu">mdholl@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Adam Lechner</td>
<td><a href="mailto:adamlechner@ksu.edu">adamlechner@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Micah Mabin</td>
<td><a href="mailto:micah.mabin@und.edu">micah.mabin@und.edu</a></td>
<td>University of North Dakota</td>
</tr>
<tr>
<td>Noelhala Monzon</td>
<td><a href="mailto:noahlanam@hotmail.com">noahlanam@hotmail.com</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Shane Nichols</td>
<td><a href="mailto:shane.nichols@nyu.edu">shane.nichols@nyu.edu</a></td>
<td>New York University</td>
</tr>
<tr>
<td>Shalisa Oburn</td>
<td><a href="mailto:shalisa-oburn@uiowa.edu">shalisa-oburn@uiowa.edu</a></td>
<td>University of Iowa</td>
</tr>
<tr>
<td>Manomi Perera</td>
<td><a href="mailto:manomi@ksu.edu">manomi@ksu.edu</a></td>
<td>Kansas State University</td>
</tr>
<tr>
<td>Matthew Peterson</td>
<td><a href="mailto:matt.peterson@biogen.com">matt.peterson@biogen.com</a></td>
<td>Biogen</td>
</tr>
<tr>
<td>Yue Qiu</td>
<td><a href="mailto:yqiu@chem.wisc.edu">yqiu@chem.wisc.edu</a></td>
<td>University of Wisconsin at Madison</td>
</tr>
</tbody>
</table>
Michaella Raglione  
michaella-raglione@uiowa.edu  
University of Iowa

Kamal K. Ray  
kamalkanti-ray@uiowa.edu  
University of Iowa

Molly Reinmuth  
Mollyreinmuth@gmail.com  
Kansas State University

Rachel Roccanova  
rvow@ou.edu  
University of Oklahoma

Kanchana Samarakoon  
Kanch@ksu.edu  
Kansas State University

Bhupinder Sandhu  
bhupindersandhu90@ksu.edu  
Kansas State University

Bayram Saparov  
saparov@ou.edu  
University of Oklahoma

Amy Sarjeant  
sarjeant@ccdc.cam.ac.uk  
Cambridge Crystallographic Data Centre

Nandini Sarkar  
nsarkar@ksu.edu  
Kansas State University

Chris Satterfield  
csatter@ksu.edu  
Kansas State University

Dylan Shields  
shielddj@mail.uc.edu  
University of Cincinnati

Abhijeet Sinha  
sinha@ksu.edu  
Kansas State University

Weiwei Tang  
tang248@purdue.edu  
Purdue University

Jesus Valdes-Martinez  
jvaldes@iquimica.unam.mx  
National Autonomous Univ. of Mexico

Bo Wang  
wangbo@ksu.edu  
Kansas State University

Zijun Wang  
zijun.wang@und.edu  
University of North Dakota

Shweta Yelgaonkar  
shwetapandharinath-yelgaonkar@uiowa.edu  
University of Iowa

Fudan Zheng  
zheng391@purdue.edu  
Purdue University