American Crystallographic Association Video Library
an AIP Venture Grant Supported Project

Allen G. Oliver, Karen C. Glass, Matthew L. Brown, Yinka Olatunji-Ola, Tiffany L. Kinnibrugh, Charlotte L. Stern, Alain Beauparlant, Christine Zardecki, Michael M. Aristov, Kristin Stevens

Purpose & Plan

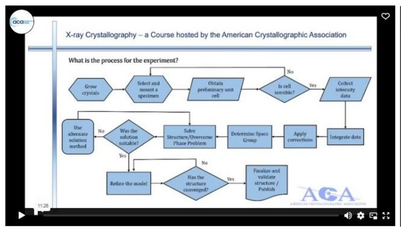
A central goal of the ACA is to "advance, promote and preserve crystallography, structural science, and allied disciplines for the benefit of humankind" (https://acas.memberclicks.net/statements-policies). Over the years the ACA has strived to meet this goal with publications, conferences, and public outreach. In 2018 the ACA launched a new website with the goal of continuing to share Structural Science.

The ACA Video Library (AVL) is building educational content for structural analysis. We are excited to share progress with this ongoing initiative which has been made possible by the generous support of the AIP and the Venture Grant Program.

Inspiration & Catalog

The complete catalog has been established and the Education Committee continues to strive to fill this page with educationally relevant videos relating to structural science. The website will be available to all.

An Introduction to Crystallography



A Hands-on Guide To Instrumentation

Crystallographic Literacy and Understanding

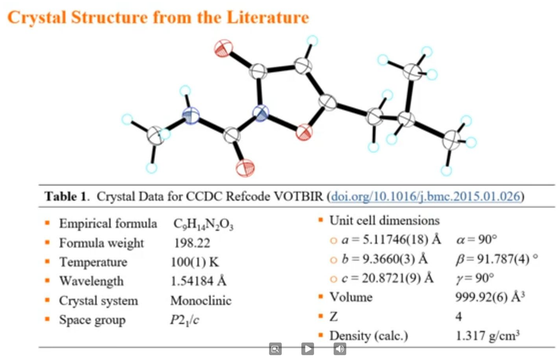

Crystal Structure from the Literature

Table 1. Crystal Data for CCDC Refcode VOTBIR (doi.org/10.1016/j.bmc.2015.01.026)

Empirical formula	$C_9H_{14}N_2O_3$	Unit cell dimensions	
Formula weight	198.22	$a = 5.11746(18)$ Å	$\alpha = 90°$
Temperature	100(1) K	$b = 9.3660(3)$ Å	$\beta = 91.787(4)°$
Wavelength	1.54184 Å	$c = 20.8721(9)$ Å	$\gamma = 90°$
Crystal system	Monoclinic	Volume	999.92(6) Å^3
Space group	$P2_1/c$	Z	4
		Density (calc.)	1.317 g/cm^3

Student Submitted Presentations

Sreya Paladugu: Total Scattering Analysis of Nanoparticles

There is a false belief that crystallographic analysis has become an automated process. As such, structural analysis education is primarily at the graduate level; it is uncommon or non-existent at the undergraduate level. It is true that automated single-crystal diffractometers now produce small-molecule structures quickly and with minimal training for their operators; likewise, the percentage of incorrect structures is dropping as the software improves. However, analysis is not automatic for protein crystallography, powder diffraction crystallography, pair distribution function analysis, or cryo-Electron Microscopy. The quality of structures even from automated instruments is questionable without inspection and supervision by a well-trained crystallographer. There is a significant knowledge gap in what is going on in "the black box".

The lack of educational resources for students, in the U.S.A. and internationally, presents both a challenge and an opportunity for the American Crystallographic Association. The ACA Summer School offers a week of training in small molecule structure determination, and powder diffraction techniques. There are other short-duration course and workshops, where each allows researchers to get started with crystal structure analysis. However, these courses do not give them the experience to solve hard problems or notice sophisticated mistakes.

From where will the next generation of experts come? In the words of Cornell Professor Nozomi Ando: *as the techniques become more advanced, the gap between what is normally taught in classes (theory) and what is needed in practice becomes larger*.

Goals & Submissions

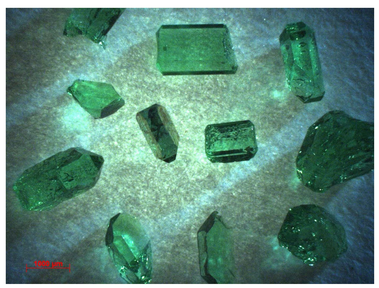
The primary goal of the project is to provide reliable, well-informed educational resources for anyone interested in structural science.

Videos can be as simple as a few minutes of talking over a slide presentation, or as complex as a molecular animation. We are starting quarterly initiatives to encourage submissions along certain themes.

Further information is available at :
https://www.amercrystalassn.org/video-library

We are now accepting submissions to the AVL. Some of the topics we are interested in (but not limited to) include:

- Historical perspective
- Crystallization/ what can we glean?
  - How to grow a good crystal
  - Visual inspection
    - Size, shape, crystallinity
  - Confirmation of synthetic process
  - Three-Dimensional imaging of your molecule in the solid state
  - Connectivity
  - Stereochemistry
  - Packing considerations
    - Void spaces
  - Distances, angles, torsions
  - Intermolecular interactions
    - Hydrogen bonding
    - Pi-stacking
  - Phase Problem
  - Data Collection
  - Structure Solution
  - Model Refinement
  - Synchrotrons
  - X-ray Free Electron Lasers
  - Electron Diffraction methods
  - Finalizing your report
  - Publishing your structure
  - Diffraction theory
    - Bragg's Law
    - Ewald Sphere and Reciprocal Space



Challenges Encountered During the Project

The most significant challenge is building the library. Volunteer submissions to the project has proven to be a hurdle. Developing the portal has involved a considerable effort on the part of our webmasters (AB, MMA). However, with the portal in place we are confident that video submissions will steadily appear, and this will become a valuable resource for the greater community.