Seeing is Believing
– How Can Crystallography and X-Ray Diffraction Help?
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X-Ray Laboratory at Harvard:
Our X-Ray laboratory provides access to the state-of-the-art equipment and technologies, holds crystallography course (Chemistry 255: Practical Crystallography in Chemistry and Materials Science) and X-Ray diffraction application training, and offers advice and technical assistance in crystal growth, data collection, and structure refinement. Our facility opens to all Harvard members, as well as external users.

Instrumentation:
- APEX II DUO
- D2 PHASER
- D8 DISCOVER

Our X-Ray laboratory has two Bruker APEX II DUO CCD single crystal diffractometers, both equipped with Mo/Cu radiation sources and Oxford Cryosystem700 series low temperature devices. We provide:
1) Routines small molecule crystal structure determinations (up to 500 non-hydrogen atoms, at 80-400 K);
2) Absolute configuration determination for biologically active compounds that only contain C/N/O atoms;
3) Charge density analysis, including ultra-high resolution, ultra-low temperature data collection (~10 K), and multipole refinement, combined with theoretical calculations;
4) Photo-crystallography study in exploring molecular meta-stable states;
5) Resonant diffraction studies/Diffraction anomalous fine structure.

Our X-Ray laboratory also has a Bruker D2 PHASER and a D8 DISCOVER with DAVINCI-Design X-Ray powder diffractometer. The D2 PHASER is a novel desktop X-Ray diffraction tool enabling fast data collection for phase identification and Rietveld refinement; while the D8 DISCOVER with DAVINCI-Design is equipped with both a zero-v首都的 LynxEye detector and a two-dimensional VANTEC-500 detector. It is capable of performing:
1) Qualitative and quantitative phase analysis;
2) X-Ray reflectivity and high-resolution X-Ray diffraction analysis of thin films;
3) Stress measurement, texture analysis and phase identification on the sample with even only 0.5 mm diameter area.

The extra MRI temperature stage provides a wide range sample environment, from -180 to 1,400 Celsius.

Small-Molecule Crystallography Service:

Why crystallography?
Crystallography is the experimental science of determining the arrangement of atoms in crystalline solids. – From Wikipedia
Crystalline means that the solid has three-dimensional periodicity - after a certain distance, the same structure repeats itself in every direction.

Crystallography provides an unambiguous result:
- Location and type of atoms, bond distances/local environment;
- Absolute structure.

Structural Dilemma – Isomers:

Structural Dilemma – Absolute Configurations:

Structural Dilemma – Meta-Stable States:

X-Ray Diffraction Service for Thin Film and Powder Samples:

Why X-Ray Diffraction?
X-Ray diffraction is an easy and fast way to obtain fundamental information about the structure of a crystalline material, including thin film and powder samples.

Thin Film Thickness Determination:

Non-Destructive Phase Identification:

Location:
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“to service, to educate, to enable!”