[**Center for Crystallographic Studies (X-Ray Laboratory)**](http://chemistry.harvard.edu/pages/x-ray-laboratory)

**URL:** <http://chemistry.harvard.edu/pages/x-ray-laboratory>

**Faculty Director:** Theodore Betley

**Technical Director:** Shao-Liang Zheng

**Description:**

*Square Footage: 2,051*

*Address:**12 Oxford Street, Bauer B04-06, Cambridge, MA 02138*

The X-Ray diffraction facility in provides access to state-of-the-art equipment and technologies, hosts a [crystallography course](https://chemistry.harvard.edu/pages/x-ray-laboratory#education) and X-Ray diffraction application training, and offers advice and technical assistance in crystal growth, data collection, and structure refinement.

Our facility has a [Bruker](http://www.bruker.com/) D8 VENTURE equipped with PHOTON-100 CMOS detector, high brilliance Mo/Cu IµS microfocus X-ray sources, and [Oxford Cryosystream](https://www.oxcryo.com/product/cryostream-800) 800 series low temperature device. And two APEX DUO single crystal diffractometers equipped with APEX II CCD detector, Mo (Triumph)/Cu (IµS microfocus) X-ray sources, and Oxford Cryosystream 700 series low temperature device.

Our facility provides routine small molecule (up to 500 non-hydrogen atoms) crystal structure determinations (80-400 K), including determinations of the absolute configuration of biologically active compounds, which often do not contain atoms with larger resonant scattering signals than that of oxygen.

The X-ray laboratory is regularly awarded beam time from the Advanced Photon Source (APS) Argonne National Lab for micro-crystallography studies, high-resolution charge density studies, photocrystallography studies, and resonant diffraction studies.

The X-Ray diffraction facility also offers analyses of powder samples and thin films. The laboratory has a [Bruker D2 PHASER](http://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/x-ray-diffraction/d2-phaser/overview.html) and a [D8 DISCOVER](http://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/x-ray-diffraction/d8-discover/overview.html) with DAVINCI design X-Ray powder diffractometer. The [D2 PHASER](http://chemistry.harvard.edu/files/chemistry/files/d2_phaser_doc-b88-exs017_en_high.pdf) is a novel desktop X-Ray diffraction tool enabling fast data collection for phase identification and Rietveld refinement. The D8 DISCOVER with DAVINCI design is equipped with both a zero/one-dimensional LynxEye detector and a two-dimensional VÅNTEC-500 detector. It is capable of performing X-Ray diffraction on powder samples, as well as X-Ray reflectivity and high-resolution X-Ray diffraction analysis of thin films.

**Equipment**

* Bruker D8 VENTURE single crystal diffractometer
* Bruker APEX II DUO single crystal diffractometer
* Bruker D2 PHASER powder diffractometer
* Bruker D8 DISCOVER with DAVINCI design powder diffractometer
* Zeiss SteREO Discovery V8 microscope with AxioVision and Polarized light applications
* [Oxford Cryosystream](http://www.oxcryo.com/coolers-for-diffraction/cryostream) 800 and 700 series low temperature device

**Services**

The X-ray facility strongly encourages user participation in structure determination and refinement and graphics interaction of molecular structure determinations. Users who wish to participate in single-crystal structure determination, powder sample measurement and thin films analysis (DIY users) may do so after taking the crystallography course (Chem255) or the X-Ray diffraction application training for powder and thin-film analysis. The current in-house instruments are [capable of performing](https://chemistry.harvard.edu/files/chemistry/files/170614_xrd_poster_for_shaoliang2.png?m=1618683838):

* Routine small molecule (up to 500 non-hydrogen atoms) crystal structure determinations (80-400 K) using single-crystal diffractometers
* Qualitative and quantitative phase analysis by using Bragg-Brentano focusing with LynxEye geometry on the powder diffractometers;
* High-resolution X-ray diffraction and X-ray reflectivity (HRXRD/XRR) analysis of thin-film samples by using Göbel mirror/ACC2 with LynxEye geometry on the D8 Discover powder diffractometers;
* Stress measurement, texture analysis and non-destructive phase identification on the sample with even only 0.5 mm diameter area by using 2D X-ray diffraction (XRD2) with VÅNTEC-500 geometry D8 Discover powder diffractometers.

**Education and Outreach**

We welcome students from all levels—high school, undergraduate, graduate and post-graduate—to our X-ray laboratory. Visitors will learn about X-ray science and instrumentation through hands-on activities.