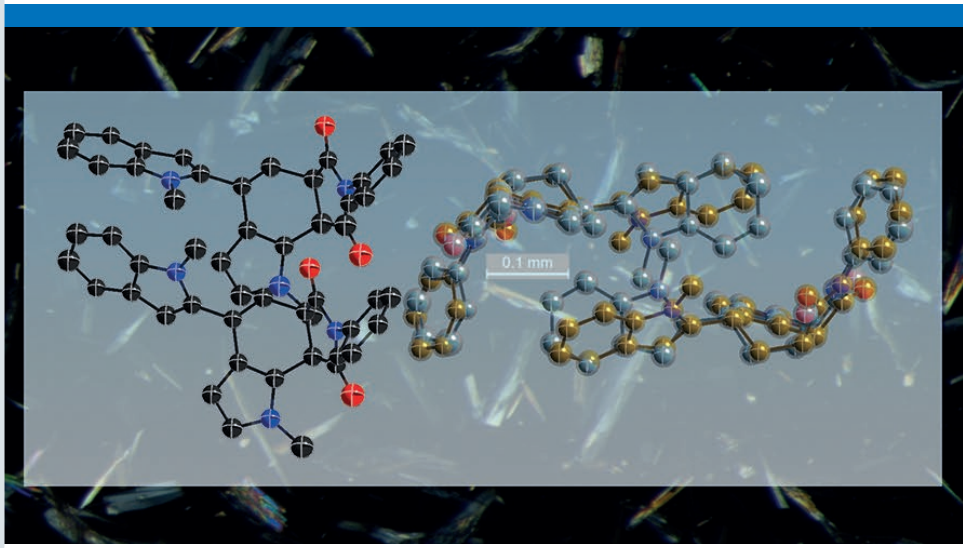
"The PHOTON III detector has provided the tools to acquire data on the most difficult specimens for laboratory crystallography at the University of Minnesota including very small organics to incommensurately modulated materials."

Dr. Victor G. Young, Jr., University of Minnesota



Case Study 7
Upgrading to the Photon Counting PHOTON III Detector

Executive Summary

The PHOTON III detector realizes the full promise of photon counting with CPAD technology.

- Delivers zero-background mode
- Eliminates zingers arising from ubiquitous radioactivity
- Provides long acquisitions on the smallest specimens

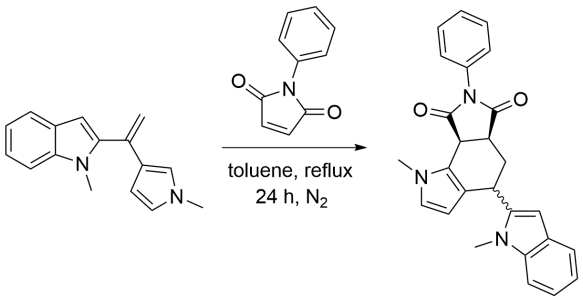
Challenges

Our graduate students and postdoctoral researchers continually supply the most challenging specimens for small-molecule crystallography. The specimens typically include high Z' light-atom structures with extremely large unit cells, twinned or incommensurately modulated structures or crystals.

The Upgrading Experience

Our D8 VENTURE Kappa diffractometer was equipped with Cu- and Mo-microfocus sources and a PHOTON II detector prior to the upgrade. The detector upgrade was easily accomplished with a simple swap of the detector data-processing unit. The PHOTON III significantly improves our ability to index and collect proper data sets from our challenging samples.

We now rarely travel to the synchrotron to collect data for these samples, since we can give researchers the data they need to publish their work.



endo/exo
78%/8%

A Challenging High Z' Organic Compound Example

The endo- and exo-isomers resulting from the [4+2] cycloaddition above were separated chromatographically but yielded very small needles and plates. Even the largest specimen diffracted poorly. Our PHOTON III detector allowed collecting a full data set to ~1.0 Å resolution using exposure times as long as 3 minutes per frame. The resulting structure is shown in the top banner. The high Z' asymmetric unit contains four molecules: Two are related by partial translational symmetry (left), while the other two exhibit whole-molecule disorder (right). For this diastereomer the methylindole substitutional group was found to insert on the exo-face.

We are grateful to the Noland Group at the University of Minnesota for providing the reaction scheme.