

The Rigaku XtaLAB Mini for use across the undergraduate curriculum to teach single crystal x-ray crystallography

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Single crystal X-ray crystallography is utilized to determine the solid-state structure of a molecule. In spite of this, single crystal X-ray crystallography is not taught at the undergraduate level in most colleges/universities. A conceptual coverage of single crystal X-ray crystallography may occur in upper level classes, but usually the experimental part is ignored. Most graduates lack experience in single crystal x-ray crystallography upon conferral of their American Chemical Society (ACS) Chemistry degree. Graduates go to graduate school, or the workforce, underprepared. We developed a way to address and resolve this lacuna. Diffraction experiments that span the undergraduate curriculum challenge students at each educational level and prepare them for life after a Chemistry B.Sc. The experiments increase in difficulty level from the sophomore to senior level. For example, the X-ray structure of sucrose can be solved from crystal selection to preparation of an ORTEP in a senior class. In a sophomore level class, students can use pre-reduced data to solve the structure. When one undergraduate laboratory experiment is vetted at the senior level, this experiment is adapted to the junior level and a new experiment is introduced at the senior level. In two-to-three years, a complete set of experiments cover the laboratory course curriculum. Assessment of these experiments will include sharing the curriculum with predominantly undergraduate institutions 500 miles around ETSU. The curricular redesign will be shared at both ACA and ACS meetings. We plan to share this curriculum with the Committee on Professional Training (CPT) of the ACS (the CPT determines the minimum criteria for an ACS approved degree). We anticipate that these experiments will be well received, both by the ACS community at large and ACS-CPT.