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Pappenfus, University of Minnesota, Morris associate professor of chemistry, among consortium of researchers awarded National Science Foundation funds for regional molecular structure facility

Summary: Five colleges and universities will share a single-crystal X-ray diffractometer for research training and education in chemistry and materials research.

(August 30, 2011)-Ted Pappenfus, associate professor of chemistry at the University of Minnesota, Morris, is a member of a consortium of researchers that received a National Science Foundation (NSF) Major Research Instrumentation (MRI) Program award. With this award, Pappenfus and colleagues from the College of St. Catherine, Carleton College, the College of St. Benedict, and St. John's University will acquire a benchtop X-ray diffractometer for a regional molecular structure facility.

"An X-ray diffractometer allows accurate and precise measurements of the full three dimensional structure of a molecule and provides accurate information about the spatial arrangement of a molecule relative to neighboring molecules," Pappenfus explains. The \$201,787 award covers the instrument, microscope, and training by the manufacturer. The equipment will reside at St. Catherine's, and access will be reserved online.

Pappenfus credits the established relationship between the co-principal investigators and the appeal of a consortium of users, embodying cooperation and cost-consciousness, for their success in winning the grant on their first try. And it signifies innovation for the consortium members, allowing them to do what they could not do alone while saving money.

The impact of the award, Pappenfus summarizes, is removing limits on what the researchers can do with regard to understanding the structure of materials. It will enhance research training and education, augmenting his teaching as X-ray crystallography is becoming a more routine technique, especially at the undergraduate level, with advances in both software and equipment. A personal advantage is also likely, he says: "I think I'm going to learn a lot because I'm familiar with the technique from afar. Now I'll get hands-on experience, and that's when you really start learning."

Pappenfus's research requires the ability to grow quality crystals to determine the structure of a molecule. He and his students will use the instrument in organic materials research to reveal the 3-D structure of the materials they are working with. "Because structure dictates properties," Pappenfus clarifies, "researchers need to know the structure-property relationships when making molecules. This equipment will enable us to confirm that we made what we intended." His first new project with his students will be making new materials for organic solar cells to determine if they are good candidates for solar energy conversion.

Speed also powers this technique. Under the old scenario, Pappenfus and his students might make a molecule one day and results could take several more days to months, delaying progress and depleting research budgets. Data derived from the University's existing equipment must be shipped to the Twin Cities campus for analysis at a cost of up to \$600 per sample. The researchers will soon be able to do their own analysis on site at St. Catherine's at no cost, and data can also be collected remotely. But the most exciting difference between this and current equipment available at UMM, Pappenfus reiterates, is in removing doubt in the absolute structure determination of molecules and confirming those

important structure-property relationships, elevating the analysis to the next level.

Pappenfus obtained a bachelor of arts in chemistry from St. John's University and earned a doctorate in inorganic chemistry from the University of Minnesota. His teaching and research focus on organic materials and inorganic chemistry.

Below: Crystal structure of a molecule prepared by undergraduate student Dan Seidenkranz '13.

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