

Single Crystal Photocrystallography – Watching Chemistry Happen

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For the last 100 years single-crystal X-ray crystallography has been undisputedly the best way of determining the full 3-D structure of a crystalline material. However, until recently, the method did not provide direct evidence of the reactivity, effectively providing only a snapshot of the structure of the starting material or the reaction product. This situation has changed over the last two decades because of the power of synchrotron radiation, coupled with advances in cryogenics, detector technology and laser systems, and the science of “photocrystallography” has been born.¹ This technique provides the ability to determine the structures of short-lived or metastable species within the crystalline environment when crystals are irradiated by light. There are many important chemical processes that occur on time scales ranging from nanoseconds to hours that can now be probed crystallographically,² providing valuable information on the way that molecular sensors and photocatalysts work.

We will present an overview of the area of photocrystallography as applied to molecular systems, particularly highlighting the research on metastable and short-lived species that has been carried out on beamline I19 at Diamond, and putting this into the context of worldwide research in the area. The systems studied at Diamond include transition metal linkage isomers that switch coordination mode upon photoactivation. It is possible to monitor and visualize this switching processes within the single crystals and to obtain solid-state kinetics on the reactions.^{3,4}

The possibilities for studying processes in molecular crystalline complexes that occur on the nanosecond timescale will also be discussed.

References

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