



Technical Staff and PI Prof Murugavel (middle) in front of the new D8 QUEST.

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Prof. Murugavel, Department of Chemistry at IIT Bombay

Just a few days after Bruker's service engineers installed our new D8 QUEST, we received an impressive training on the APEX3 software suite by Bruker's Application Specialist. The APEX3 suite is an integral part of Bruker's SC-XRD solution. We are extremely pleased with the performance of the D8 QUEST hardware. Already prior to the training we were very positively surprised that the executables for SHELXS and SHELXL programs, written by Prof George Sheldrick, were included with the suite, eliminating the need to obtain these programs from third-party sources.

During the two-day training, we collected data from a couple of samples of both organic and metal-organic compounds and gained a deep insight into the program flow of the APEX3 software suite, from mounting the sample to final publication of the structure (graphics and CIF file). The new default matrix strategy (FAST SCAN) adopted in APEX3 proved to be extremely useful, as within a short time we were able to check the crystal quality, determine the unit cell, and even obtain a preliminary structure. The latter is hugely helpful for quickly deciding whether to continue data collection or not. The space group symmetry obtained during the new matrix strategy helped us determine the best strategy for data collection and avoid any symmetry-related bias. APEX3 structure solution routines are extremely powerful and the subsequent model building and refinement can be easily accomplished with the SHELXLE routine provided within the suite.

We are really impressed by APEX3's large number of well-tested engines and routines. Bruker developers managed to arrange this wealth of programs into an easy-to-use software suite with a very clear structure and program flow. The package allows easy sample processing, including modulated and twinned samples, for the users in the Department of Chemistry at IIT Bombay. Bruker's new IDEAL routine goes beyond the standard independent atom model (IAM) refinements and provides us with detailed insights into bond and lone-pair properties of the structure.

Our overall experience with the hardware, software, and application training has been excellent. We are looking forward to the advanced application training for the Department, which will provide us with deeper insight into the best handling of challenging structures, such as twinned samples, samples with ambiguous symmetry, and/or highly disordered structures. We are convinced that the Bruker team will look after the D8 QUEST system well in the future.

## The APEX3 Software Suite

- An easy-to-use software package with a very clear structure and program flow

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