

## Single crystal electron diffraction studies at Core Facility

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Crystallization process in many cases leads to crystals of insufficient size to solve the structure with X-ray diffraction techniques. However, recent advances and an increase in accessibility of transmission electron microscopes allows to use electron diffraction to study such specimens more prevalently. While the electron diffraction experiments come with challenges such as higher cost, reduced convenience regarding the sample preparation and crystal testing, there are some areas where this technique is more advantageous. One of such assets is identification of hydrogen atoms presence. Routine X-ray measurements hardly ever provide electron density maps that allow to distinguish high enough peaks to allocate hydrogen atoms, while the typically collected electron diffraction data seems to allow to overcome this problem much more often. What is worth noting, the electron diffraction studies provide much more reliable positions of hydrogen atoms and these are usually quite consistent with neutron studies.

Even though the electron diffraction technique is not as well established as X-ray diffraction, the rapidly developing instrumentation and software allows for better quality studies than before. As the typical electron diffraction measurement covers only a small fraction of the Ewald sphere, solving the structure often is problematic for low symmetry systems. To overcome such difficulty, it is useful to collect a few sets and combine them together to get higher completeness of the data for the final model. This is not performed just for the sake of better statistics but in many cases is a vital part of determining the real space group of the examined compound.

In the main part of the poster, we show several cases from our research where small-molecule compounds could not provide crystals of sufficient size for X-ray diffraction measurement but were of ideal volume to conduct electron diffraction experiments. In our studies we used independent atom model with the common kinematic approach where the dynamical effects are accounted just by applying the extinction correction. Such a simple approach is often sufficient to obtain a sensible model even though the statistics such as  $R_1$ ,  $wR_2$ ,  $R_{int}$  or mean  $I/\sigma$  look much worse than expected. To expand the topic even more, we would like to also show a few cases where the X-ray diffraction data were available and the comparison between the models obtained from both methods was possible.

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