

Still Bad Crystals, but Good Data and Results from Synchrotron Facilities

William Clegg, Ross W. Harrington, School of Natural Sciences (Chemistry), University of Newcastle upon Tyne, NE1 7RU, U.K.. E-mail: w.clegg@ncl.ac.uk

In many cases it is simply not possible to transform bad crystals into good ones, but a crystal structure is still required. The use of high-intensity synchrotron radiation can overcome some of the problems, particularly weak diffraction, whether this be a result of small crystal size or of structural faults such as disorder or twinning.

For real success, dedicated single-crystal facilities are needed, optimized for this application and using good quality X-ray optics, state-of-the-art diffractometer and detector systems, and usually low-temperature equipment. The "small-molecule" diffraction station at Daresbury SRS, constructed about 10 years ago, has been a spectacular success with great productivity and a high level of oversubscription by users, and a second station is now available.

More recently the facility has been used for a national crystallography service for UK chemistry research groups, providing rapid access and expert staffing. As many as 12 data sets per day have been measured from samples that are known to be beyond the capabilities of the most powerful rotating-anode area-detector chemical crystallography system in the country (perhaps in the world) and have been brought to us as a last resort. Although some samples really are beyond hope (including those that simply aren't crystalline at all), the majority have yielded their inner secrets, though the effort involved is often considerable when twinning, disorder, pseudosymmetry and other challenges have to be faced.

Keywords: **synchrotron x-ray diffraction, structure determination, service crystallography**