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A high-flux synchrotron station for single-crystal diffraction

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Summary

A new single-crystal diffraction station has been designed, constructed, and commissioned at Daresbury Laboratory Synchrotron Radiation Source, for structure determination in chemistry and materials science.

The station, denoted 9.8, utilises synchrotron radiation from an existing wavelength-shifting wiggler magnet (beam-line 9); this is focused horizontally and a single wavelength selected by a bent triangular monochromator, and focused vertically by a bent planar mirror. A modified Enraf-Nonius CAD4 diffractometer is available for special requirements such as high-pressure studies. Most diffraction measurements are made with a Bruker AXS SMART CCD area-detector system with integrated goniometer. These instruments are mounted on an alignment table and are controlled from an adjacent user area, which also provides facilities for sample mounting, including the handling of air-sensitive materials and examination with a high-power microscope, and for data processing, structure solution and refinement, and the transfer of data and results to users' home institutions. The design specifications of the station have been met and exceeded.

Commissioning of the station with user-supplied samples has involved collaboration with many research groups and the examination of a wide variety of molecular and non-molecular materials, which it has not been possible to study by conventional laboratory techniques. These include supramolecular assemblies, complexes of macrocyclic and other large ligands, polynuclear metal clusters, microporous catalytic materials, extended arrays for special electronic and magnetic applications, pigments, liquid crystal precursors, bioinorganic and bioorganic compounds, and pharmaceuticals. Most data have been collected at low temperature; some experiments have been at elevated temperatures or at high pressure. Anomalous dispersion effects have been exploited by wavelength tuning, and high-resolution data have been measured for charge density studies.

Results have been published in leading journals, and many further manuscripts are in press or in preparation.

The new station is a world-class facility providing unique opportunities for new research, and is now a standard part of the experimental facilities offered by Daresbury Laboratory SRS.

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