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Enhanced Crystallographic Facilities for Inorganic and Organic Materials

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Summary

A CCD-based area-detector diffractometer has been installed to extend the capabilities of existing crystallographic equipment, both in terms of volume and in dealing with more difficult samples. Newcastle was the world's first customer for the new Siemens SMART system in 1994.

The equipment has been used to collect over 850 single-crystal diffraction data sets in 2.5 years since its installation. Advantages over conventional four-circle diffractometers include the faster collection of data, especially for large structures; the ability to obtain data from samples of poorer quality, particularly those giving weaker diffraction intensities; the very rapid preliminary screening of samples; and the high degree of redundancy and symmetry-equivalent reflections achieved in most data sets.

Over 50 publications have appeared so far, describing about 100 of the determined structures. A further 100 structures are in papers which are either in press or in preparation. Work has been presented at several national and international meetings, where both the structural results and the application of the CCD technology have attracted considerable interest.

Previous collaborative projects have been continued and extended, and several new ones have been established, taking advantage of the much increased capacity and the enhanced capabilities of the new equipment. Major projects include: (1) metal oxides and polyoxometallates, with applications in sol-gel processing, catalysis and electro ceramics; (2) ligands designed for selectivity of particular metals, including biomimetic studies; (3) complexes of ligands incorporating nucleobases, with the aim of designing properties of coordination and intermolecular interactions; (4) transition metal allenyl complexes, with applications in target synthesis and catalysis; (5) organic synthesis reagents, particularly for regio- and stereoselective reactions; (6) bio-organic and medicinal chemistry; (7) compounds of *s*-block elements, and the use of some of these as intermediates in the synthesis of lanthanide complexes of bulky ligands; (8) imido and calixarene complexes; (9) metal thiolates and related complexes, including models for biological systems; (10) boryl compounds and the role of their metal complexes in catalysis, especially for diboration reactions; (11) molecular structures and intermolecular interactions of rigid-rod organic compounds with liquid-crystal, non-linear optic, and other special properties; (12) macropolyhedral boron-containing cluster chemistry.

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