MS36 P01

Crystallography with a dual source diffractometer at Reading. Yu Gan[a], R. Jeremy H. Davies[b], Anna. L. Brogden[a], Abeer Naseer[a], Sayima. J. Ahmed[a], Christine. J. Cardin[a]. [a]*Department of Chemistry, University of Reading, RG6 6AD UK.* [b]*School of Biological Sciences, Queen's University, Belfast BT7 1NN UK*
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Keywords: copper source, absolute configuration, DNA

A newly installed diffractometer with facile switching over between copper and molybdenum sources has made the crystallographic studies at Reading more versatile, and this poster demonstrates this with some recent results. The R_{int}s of the data collected with the molybdenum source very often stay at around two percent, which makes the structure solution for difficult structures become possible. On two occasions where Br^- or I^- were included in the structure as counter ions, the absolute configuration of the chiral molecule was determined with very reliable statistics. On the other hand, with a focused copper source also available, the determination of the absolute configuration of typical organic molecules can be routinely carried out. An excellent example is the high resolution crystal structure of the intramolecular thymine-adenine photoadduct d(TpA)* (Figure 1), in which the absolute configuration at the original thymine C5 and C6 atoms confirm the hypothesized photoaddition mode that should be favored by the stacked thymine and adenine bases in B-DNA. All hydrogen atoms were readily located. [1] The stronger copper source also makes it possible to study structures of supramolecular crystals, which very often have tiny crystal sizes. These crystals, as well as being tiny, often have cell dimensions extending to 40-50Å or more, when the long wavelength of copper makes the diffraction spots better resolved. For the same benefits, studies on DNA structures and their interactions with small ligands, and protein crystal engineering utilizing lysozyme and thaumatin as the subjects are also carried out. Nice results like DNA-intercalator complexes, DNA Holliday junctions formed by new sequences, and new A-DNA structures are obtained on a regular basis.

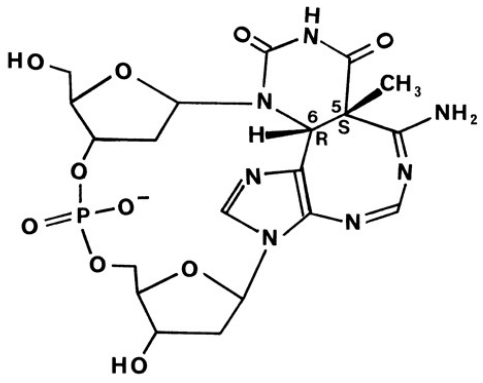

Figure 1 Structure of d(TpA)*

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MS36 P02

Experiences with a High-Brilliance Microfocus Sealed Tube Juergen Graf, Carsten Michaelsen, Christian Hoffmann, *Incoatec GmbH, Max-Planck-Straße 2, D-21502 Geesthacht.* E-mail: info@incoatec.de

Keywords: X-ray optics, multilayer thin films, new XRD technology

With the gaining importance of macromolecular crystallography came an increasing need for highly intense X-ray sources enabling the analysis of very small and weakly scattering samples. High-brilliance microfocusing X-ray sources are characterized by high power loads in spot sizes of ≤ 100 μm at the anode and deliver an intense but divergent beam which demands for the use of an X-ray optics. Synthetic multilayer mirrors are well established as excellent beam-shaping devices with a very good spectral purity [1, 2, 3, 4]. Their high reflectivity, broad rocking curve and tunable beam divergence and cross-section make them the ideal focusing optics for conserving the source brilliance [5, 6].
New microfocusing sealed tube X-ray sources, such as the *Incoatec Microfocus Source* (IμS^{TM}), are low-maintenance high-brilliant sources which significantly improve the performance of home-lab instruments when combined with dedicated multilayer mirrors. IμS^{TM} contains a 30 W air-cooled microfocus sealed tube with high brilliance and a high-performance 2D Montel multilayer mirror. IμS^{TM} is available for Cu-K_α and Mo-K_α radiation
We will present results on the use of IμS in protein and small molecule crystallography and in small angle X-ray scattering which show that the performance of such an air-cooled microfocusing sealed tube is much better than that of standard sealed tube systems and comparable to traditional rotating anode sources but with a significantly reduced maintenance.

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MS36 P03

A New Flexible High Resolution Powder Neutron Diffractometer at IFE in Norway Klaus Lieutenant[a], Bjørn C. Hauback[a], Helmer Fjellvåg[b], Phillip Bentley[c] [a]*Physics Department, Institute for Energy Technology, Kjeller, Norway.* [b]*University of Oslo, Norway.* [c]*Hahn-Meitner-Institut, Berlin, Germany.*
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Keywords: neutron diffraction; powder diffractometer; Monte Carlo treatment

Various parameters of a neutron powder diffractometer can be varied to increase the flux at the sample. Additionally or alternatively the detector area can be increased to yield a higher count rate. The increased intensity comes on the cost of resolution and precision of