



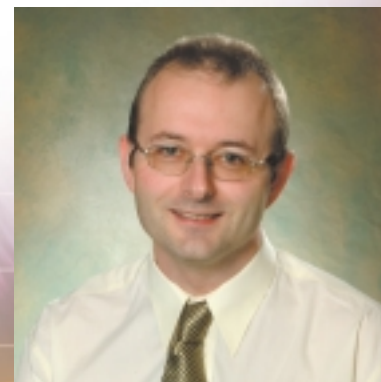
Welcome to this the second issue of our newsletter designed specifically for the chemical and speciality sector. We have decided to use the newsletter to showcase particular areas of materials investigations which have been carried out by **DARTS**, thereby keeping you up to date with our capabilities to meet your materials characterisation requirements.

In this issue we look at a **DARTS** investigation into polymorphism in an organic pigment that was resolved using our ultra-small single crystal crystallography facility and also at an example of how **DARTS** produced a crystal structure from a powder sample of a pigment which would not grow single crystals.

In both cases the power of the synchrotron was key to getting a result. If you would like to know how **DARTS** can put this power at your disposal see the **FREE** offer in the **DARTS** Challenge.

New Team Member

We are delighted to welcome a new member to the **DARTS** chemicals sector sales team. Mark Roberts has worked at Daresbury for over 4 years and has extensive experience in powder diffraction, a technique used for many **DARTS** customers, especially in the chemicals sector.



DARTS Challenge - Get a FREE Consultancy

Why not challenge **DARTS** to solve your most pressing materials characterisation? We will give you a **FREE** consultation on the material structure determination of your choice. Just contact **DARTS** and ask for your **DARTS** Challenge **FREE** consultation.

Want to find out more?

To contact us call
or fax
or email

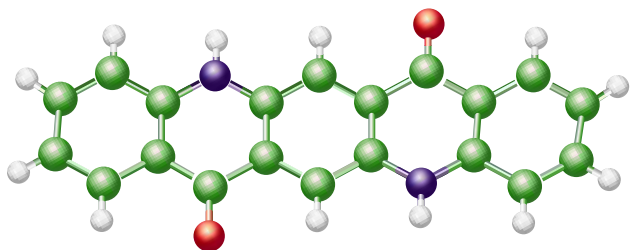
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Crystal Clear Colours

DARTS Explores the Structures of Pigments

To fully understand the colour properties of a pigment it is vital to know the crystal structure. Since an inherent property of a useful pigment is small particle size, traditional approaches to obtaining crystal structures are not always possible. This is where the properties of synchrotron radiation can be exploited. The X-rays produced from the Synchrotron Radiation Source (SRS) at **DARTS** are much more intense than those produced from a conventional laboratory X-ray generator. This means that it is possible for **DARTS** to look at much smaller crystals using the SRS.



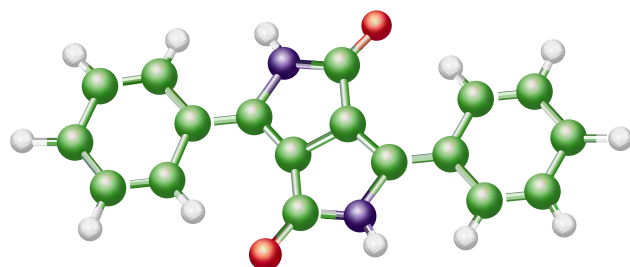
Schematic representation of quinacridone

ICI scientists looked at the problem of polymorphism in quinacridone pigments using single crystal diffraction at the SRS. The quest was to decide whether or not the two different colour forms of quinacridone were true polymorphs or not. The two forms certainly produced different powder diffraction patterns but, having determined the crystal structure of one sample, it proved possible to simulate the two powder diffraction patterns from the same structure by changing the average crystallite size - the samples were not polymorphs but polytypes.

DARTS can also solve the structures of pigments from powder diffraction data,

a relatively new technique compared with single crystal structure solution. Whilst it is possible to solve structures from powder diffraction methods using standard laboratory based diffractometers, the low symmetry of many organic materials can make analysis of the patterns difficult due to severe peak overlap. The high-resolution data obtainable on the SRS can help to overcome this problem.

One example of this type of research has been done by Ciba scientists who are interested in studying a class of pigments known as diketopyrrolopyrroles (DPPs). DPP pigments are used extensively because of the range of colours possible by simply selecting different substituents on the phenyl rings. For some samples it has proved impossible to produce single crystals so, using structure determination from powder diffraction, the packing properties of derivatives have been resolved.



Schematic representation of DPP

Recent advances in synchrotron radiation technology and in analysis procedures have significantly enhanced the understanding of pigment technology. With the limits on crystal size getting smaller, and the methods for structure determination from powders improving constantly, this is an area where **DARTS** can add value to the product development process – not only in the case of pigments but also for any crystalline material.

For information on how DARTS can help your R&D programme contact us today.