
Keywords: instrumentation, techniques for crystallisation.

Chemical crystallographers often rely on crystals provided by colleagues, who may not appreciate the dramatic influence of crystal quality on the precision of the resulting structure determination. Good communications are therefore essential. However, there is always great scope for a misunderstanding, as even apparently simple terms such as “recrystallisation” have different connotations for the participants in the dialogue. The methods used to obtain crystals for structure determination are sometimes simple adaptations of the procedures used for synthesis and purification but the former comprise a much wider range of techniques.

As a result chemists may not be aware of methods which could be highly appropriate for their compounds. The aim is always to establish a dialogue, to which the crystallographer contributes general knowledge of relevant methods, with the chemist providing specific information about the properties of their compound, for example regarding its solubility in various solvents. The outcome of such an interchange can be very positive: in one example a large research group adopted as their standard method a particular technique of which they were previously unaware but which they found to be highly appropriate and effective.

The poster will describe some of the less usual techniques which have proved successful in giving diffraction-quality single crystals.

Microgravity protein crystal growth: a case of a collagen-like polypeptide. A. Zagari1, R. Berisio1, G. Sorrentino1, L. Vitagliano1, L. Carotenuto2, C. Piccolo2, L. Mazzarella1. 1Centro di Studio di Bio cristallografia, CNR and Dipartimento di Chimica, Università di Napoli “Federico II”, Via Mezzocannone 4, 80134 Napoli, Italy, 2Microgravity Advanced Research & Support Center (MARS), Napoli, Italy.

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In the past years we have analysed the structural features of one of the most studied collagen model polypeptides (Pro-Pro-Gly)10 [1]. The study was limited due to the poor quality of (PPG)10 crystals. Microgravity has proved to be a tool for improving crystal quality by reducing the convection effect and sedimentation. Microgravity crystal growth of (PPG)10 was carried out in the Advanced Protein Crystallization Facility [2] during the STS-95 Mission. The crystal growth was regularly monitored by a video observation. Crystals were successfully grown in all experiments, using both dialysis and free-interface diffusion methods. The crystal quality of (PPG)10 was assessed by X-ray synchrotron diffraction at DESY (Hamburg) and Elettra (Trieste). Microgravity grown crystals exhibited a significant improvement in terms of the resolution limit (1.3 compared to 1.7 Å). Furthermore, the diffraction pattern showed weak reflections, never registered before, that were consistent with new cell parameters, a=26.9, b=26.4, c=182.5 Å [3]. This allowed us to derive a new model for the arrangement of the triple-helical molecules in the crystals. The refinement provided also additional and accurate information on hydration and proline puckering.

During the growth process a series of images were recorded by a CCD camera at regular time intervals. The image analysis provided evidence for the crystal motion and spatial distribution [4].

References: