360 samples per day or collection of up to 130 X-ray diffraction datasets per day. Turnaround of structural data from LRL-CAT averages less than 2.3 days from the time the crystal was created and shipped to the beamline.

Keywords: automation, synchrotron, protein

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Optimising X-ray experiment strategy on-the-fly based on feedback from automated structure solution

Richard Cooper, *Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford (UK).* E-mail: richard.cooper@chem.ox.ac.uk

The EDNA framework [1] is helping us to develop and run an automated structure solution and refinement pipeline during small molecule X-ray data collections. The partial results can be used to modify the X-ray experiment strategy on-the-fly, and so target the data which provides the best possible answer to a specific problem.

X-ray experiment strategies typically optimise the time taken to collect a unique set of data (within specified limits) followed by efficient collection of data to provide maximum possible redundancy within a given time. However - if the structure can be determined and refined early in the data collection process - information can potentially be fed back to modify the data collection in order to collect the most valuable or useful data in the remaining time. Analysis of the least-squares fit of the model to the data can quickly determine the few observations which may be profitably re-measured to most improve the estimated variance of a given model parameter [2]. Extension of this analysis allows the identification of observations whose re-measurement will most improve the estimated variance of arbitrary functions of parameters (for example: distances; angles; planes; sums and differences of occupancies *etc*.).

If the crystal structure is as expected, the experimentalist can specify particular parameters or functions of interest, in order to generate an updated data collection strategy for the remainder of the experiment.

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Keywords: automated, experiment design, least-squares analysis

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In search of Nature's secrets – Controls on biomineralisation

S.L.S. Stipp,[a] T. Hassenkam,[a] K. Sand,[a] M. Yang,[a] N. Bovet,[a] L. Schultz,[a] K.E. Henriksen,[b] [a]*Nano-Science Centre, Department of Chemistry, University of Copenhagen, (Denmark).* [b]*Maersk Oil and Gas A/S, Copenhagen, (Denmark).* E-mail: stipp@nano.ku.dk

Calcite, rhombohedral $CaCO_3$, forms easily in nature, as stalagmites and stalactites, as veins in rocks, as sediments in warm seas and in pipes that distribute water to our homes. In veins, it can form large, beautiful crystals, but even in supersaturated laboratory solutions, the most favoured crystal form is the rhomb. Many organisms produce calcite, such as oysters and coral. Earthworms excrete tiny spherules, wood lice store it on their tummies and perhaps the simplest organism, one-celled algae, create exquisite platelets called coccoliths from 20 to 60 individual calcite elements that are less than a micrometer in the longest dimension. As a biomineral, calcite rarely takes the form of a rhomb. Organisms produce complicated organic molecules that adhere to the calcite surface, inhibiting growth at some sites, thus enhancing it at others. Depending on the ecological niche the organism inhabits, it can tailor the calcite to its specific needs.

We learn more about biomineralisation by studying the mineral remains of organisms and by experimenting in ideal systems, where we can control one variable after the other. The calcite atomic structure orders water in contact and even simple compounds such as ethanol, the shortest organic chain molecule that has both a methyl group and a carboxyl group, binds strongly and orders itself. Polysaccharides, produced synthetically, or extracted from cultured coccoliths, have the power to control crystallization in the manner determined by the organism. Through a multidisciplinary approach, combining skills from physics, chemistry, geology, biology and mineralogy, from experimental and theoretical directions, from the field scale to the nanometer scale, and by studying nature and designing model systems, we are getting closer to understanding the secrets of simple organisms.

Keywords: biomineralisation, calcite, polysaccharide

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Biological and environmental influence on Mediterranean corals calcium carbonate precipitation

Giuseppe Falini,[a] Stefano Goffredo,[a] Patrizia Vergni,[a] Michela Reggi,[b] Erik Caroselli,[b] Francesca Sparla,[c] Oren Levy,[d] Zvy Dubinsky,[d] [a]*Dipartimento di Chimica 'G. Ciamician', via Selmi 2 40126 Bologna, (Italy).* [b]*Marine Science Group.* [c]*Dipartimento di Biologia Evoluzionistica Sperimentale, via Selmi 3, 40126 Bologna, Alma Mater Studiorum Università di Bologna, (Italy).* [d]*The Mina and Everard Goodman Faculty of Life Sciences, Bar Ilan University, Ramat Gan 52900, (Israel).* E-mail: giuseppe.falini@unibo.it

Scleractinian coral skeletons are made mainly of calcium carbonate in the form of aragonite. The mineral deposition occurs in a biological confined environment, but it is still a theme of

discussion to what extent the calcification occurs under biological or environmental control. Hence, the shape, size and organization of skeletal crystals from the cellular level through the colony architecture, have been attributed to factors as diverse as mineral supersaturation levels and organic mediation of crystal growth. The skeleton contains an intra-crystalline organic matrix (OM) of which only the water soluble component has been chemically and physically characterized. In this work that OM from the skeleton of the *Balanophyllia europaea* and *Leptopsammia pruvoti*, solitary scleractinian corals endemic to the Mediterranean Sea, is studied in vitro with the aim of understanding its role in the mineralization of calcium carbonate. Mineralization of calcium carbonate was carried out in calcium chloride solutions containing different ratios of water soluble and/or insoluble OM and of magnesium ions. The precipitates were characterized by diffractometric, spectroscopic and microscopic techniques. The results showed that both soluble and insoluble OM components influence calcium carbonate precipitation and that the effect is enhanced by their co-presence. The role of magnesium ions is also affected by the presence of the OM components. Thus, in vitro, OM influences calcium carbonate crystal morphology, aggregation and polymorphism as a function of its composition and of the content of magnesium ions in the precipitation media. This research, although does not resolve the controversy between environmental or biological control on the deposition of calcium carbonate in corals, sheds a light on the role of OM, which appears mediated by the presence of magnesium ions.

Keywords: coral, biomineralization, organic matrix