s8.m27.p20 **Crystal Structure of Chocolate from Powder Diffraction Data.** R. Peschar, M.M. Pop, D.J.A. De Ridder, J.B. van Mechelen, R.A.J. Driessen and H. Schenk, *Laboratorium voor Kristallografie, HIMS, FNWI, Universiteit van Amsterdam, Nieuwe Achtergracht 166, 1018WV Amsterdam, The Netherlands. Email: schenk@science.uva.nl*

Keywords: Chocolate structure; SDPD; Phase transformation

We recently solved the crystal structure of the β(V)-form of chocolate and cocoa butter (CB) by SDPD. Chocolate is a greatly appreciated sweet, produced in a complicated process from cocoa and sugar. At room temperature it consists of a well-crystallised continuous CB matrix in which fine cocoa powder and sugar particles are dispersed. Its properties, like brittleness, gloss and snap, and the fast melting at body temperature providing a cooling effect, are mainly determined by the crystalline form and melting behaviour of CB.

In good quality consumer chocolate, the CB is crystallised in one of the two highest melting forms, β(V) or β(VI). Poor storage or improper production of chocolate may result in fat bloom, a whitish layer on chocolate, which is commonly associated with the phase transition from β(V) to β(VI).

Nearly three quarters of any CB consist of three mono-unsaturated triacylglycerols SOS (1,3-distearoyl-2-oleoylglycerol), POS (2-oleoyl-1-palmitoyl-3-stearoyl-glycerol) and POP (1,3-dipalmitoyl-2-oleoylglycerol). In particular SOS is known to play a major role in the crystallisation of CB into the β forms. The similarity of the powder patterns of chocolate, CB and SOS are striking when from the XRD of chocolate the sugar-part is removed, suggesting a very close relation.

Auto-indexing techniques were not successful to determine the unit cells, probably because of the predominant fingerprint area (d = 3.5 - 5.5 Å) with strongly overlapping reflections, and of the presence of long d-spacings (64 - 65.5 Å). Finally the unit cells have been obtained with an indexing routine specially written for this purpose (Peschar, to be published) and implemented in POWSIM. The cell of β(V)-CB is very similar to that of β-SOS and to our surprise the indexing figure of merit M_{20} is similar to that of a pure phase.

We first solved the structure of SOS (63 unique non-H atoms in a triclinic cell), starting from a plausible model and using the programs FOX and ORGANA. After refinement we took the SOS structure as a starting model to solve and refine the structure of β(V)-CB, introducing partial occupancies (57%) of the two end-carbon atoms of both stearin chains in order to account for the co-crystallisation of POS and POP. The SOS and β(V)-CB structures differ slightly in the oleoyl layer.

Earlier postulated SOS models show a close-packed oleoyl layer with π-π interactions at the C_9=C_{10} double bond. However, in both crystal structures of SOS and β(V)-CB a considerably different packing is found with the oleoyl-chains related via a centre of symmetry in absence of interactions between the double bonds.

Our results enable the explanation of the molecular mechanism of the β(V) to β(VI) phase transition of CB, as we will be showing at the meeting.

s8.m27.p21 **Distributed computing for crystallographic structure determination.** Kenneth Shankland, Anders J. Markvardsen and Bill David, *ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, UK. E-mail: k.shankland@rl.ac.uk*

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'The GRID' is a term used to describe a system for the sharing, selection and aggregation of computing resources spread over a number of sites. Whilst of 'distributed' computing is nothing new, the GRID will provide a stable framework that match resources to tasks on a massive scale. Our interest in the GRID has arisen from the intrinsic parallelism of many structure determination methodologies (e.g. Maxent/LLG, genetic algorithms). We have used the Entropia DCGRID [1] system to implement a small test grid of 19 non-dedicated Windows clients (ranging in CPU speeds from 350MHz to 2400MHz) and have used this to parameterise a hybrid Monte-Carlo method of structure determination from powder diffraction data [2]. Calculations that would normally take 6 months on the fastest machine are completed in less than 2 weeks on the GRID. Our understanding of the HMC algorithm has been greatly enhanced by the results of these calculations, which would be extremely difficult to carry out in any other way. We are currently investigating another GRID system (United Devices GridMP) that will allow a substantially greater number of clients to be brought to bear on problems not only in crystallography but also in application areas including molecular dynamics and neutron instrument simulation. The use of non-dedicated resources opens up tremendous opportunities for enhanced processing of crystallographic data.

[1] http://www.entropia.com
[2] ISIS 2003 Science Highlight "Optimising a hybrid Monte-Carlo search process using distributed computing".