Crystal Structure of Chocolate from Powder Diffraction Data

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We solved the crystal structure of the β(V)-form of chocolate and cocoa butter (CB). Chocolate is a made from cocoa and sugar in a complicated process. At room temperature it consists of a well-crystallised continuous CB matrix in which fine cocoa powder and sugar particles are dispersed. 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 may result in fat bloom, the whitish layer on chocolate that is commonly associated with the phase transition from β(V) to β(VI). Any CB consists for 75% of three triacylglycerols, SOS (1,3-distearoyl-2-oleoylglycerol), POS (2-O-1-palmitoyl-3-S-glycerol) and POP. In particular SOS is known to play a major role in the β-crystallisation of CB.

The powder patterns of chocolate, CB and SOS are very similar suggesting a close structural relation. Unit cells were obtained with an indexing routine written specially for this purpose by RP. The cells of β(V)-CB and β_2-SOS are very similar and, surprisingly, so are the indexing figures of merit M_{20}. We solved SOS (63 unique non-H atoms), using the programs FOX and ORGANA. After refinement we used this structure as a starting model to solve and refine the structure of β(V)-CB, employing partial occupancies (57%) for the two end-carbon atoms of both stearin chains. Our results show a considerably different packing as postulated earlier. Moreover the crystal structure gives rise to the explanation of the mechanism of the β(V) to β(VI) phase transition of CB. This is supported by the XRD of β-POS.

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