s9'.m2.o5 **Polymorph Prediction of Long-Chain Compounds**. J. van de Streek, P. Verwer, *University of Nijmegen*.
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Long-chain compounds, such as *n*-alkanes and triacylglycerides, tend to exhibit polymorphism. In *e.g*. margarines and chocolate, where long-chain compounds are the main ingredients, the overall physical properties depend on the polymorph involved. Knowledge of the crystal structures of these polymorphs is the *conditio sine qua non* for molecular modelling of these physical properties.

Long-chain compounds also have a tendency to form very thin, twinned crystals, the structures of which cannot be elucidated using conventional single crystal X-ray diffraction techniques. X-Ray Powder Diffraction (XRPD) is a good alternative, but the loss of information involved prevents *ab initio* structure elucidation.

Polymorph prediction provides us with a tool to generate possible crystal structures, which can be checked against the XRPD pattern. In polymorph prediction, the physical property being modelled is the crystal structure itself.

It will be demonstrated how the first step in the polymorph prediction process—the generation of possible crystal structures—can be made efficient for these acicular molecules, using the observation that long-chain compounds in nature form homologously isomorphous series. Results for *n*-alkanes and triacylglycerides (fats) will be shown.

Notes