Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Crystallization of the Lewis-Wahnström ortho-terphenyl model**
ULF PEDERSEN, UC Berkeley, TOBY HUDSON, PETER HARROWELL, School of Chemistry, University of Sydney — Crystallization is observed during long molecular dynamics simulations of bent trimer molecules - one of the standard models in computational studies of viscous supercooled liquids. The crystal was not anticipated, but is surprisingly simple: the three spheres that make up the rigid molecule sit near the sites of a body centered cubic lattice (the trimer bond angle being almost optimal for this structure). Interestingly, the crystal exhibits orientational disorder with molecules aligned randomly along the three Cartesian axis (an example of cubatic orientational order). While crystallization does not disqualify this model for viscous dynamics studies (it may even be valuable that the crystal is known), it illustrates the stubborn ingenuity of molecules to pack in periodic structures and questions our intuition to predict such structures. Finally, this is a rare example of crystallization of a molecular model from melt.

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Date submitted: 19 Nov 2010 Electronic form version 1.4