Abstract No. kear327

VT-XRD Study of the Liquid Crystalline Phases of Surfactant Templated Zinc Chloride

C.L. Keary, J.D. Martin* (NC State U.), and J.C. Hanson (BNL, NSLS)

Beamline(s): X7B

Introduction: Zinc chloride is known to exhibit a network structure in the melt [1]. We have recently demonstrated that the structure of this molten network can be templated with cationic surfactants (for compositions up to 80 mole % $ZnCl_2$) to yield a new class of liquid crystalline materials that we describe as metallotropic liquid crystals [2,3]. The structure of these liquid crystalline materials varies with both temperature and composition, analogous to lyotropic liquid crystals. However, unlike other known liquid crystalline materials, the structure of the zinc chloride building blocks also changes at the different compositions.

Methods and Materials: Variable temperature diffraction data were obtained using the MAR345 imaging plate detector on line X7B at the NSLS while samples were heated from room temperature up to 300 °C at a rate of 5 °C·min^{-1} for materials prepared over the composition range of 40 to 80 mole % at intervals of 5 mole %. Selected examples are shown in Figure 1. All these compositions melt to liquid crystalline phases upon heating to greater than about 70 °C.

Results and Conclusions: Previously we have determined the single crystal structures for the two lamellar crystalline phases $[C_{16}TA]_2ZnCl_4$ and $[C_{16}TA]_2Zn_2Cl_6$ ($C_{16}TA$ = cetyltrimethylammonium) [3]. Both of these surfactant rich phases also exhibit lamellar liquid crystalline structures. Increasing the zinc chloride content, with the same $C_{16}TA^+$ surfactant cation, results in materials exhibiting a bicontinuous cubic liquid crystalline structure for compositions between 52 and 65 mole % $ZnCl_2$ and a hexagonal columnar liquid crystalline phase for compositions between 60 to 80 mole %. A second cubic phase is also observed at higher temperatures at greater than 75 mole % $ZnCl_2$. Shortening the length of the surfactant tail exhibits a similar influence on the structure as does increasing the concentration of zinc chloride. The structure of $[C_8TA]_2ZnCl_4$, Figure 2, was solved from the single crystal data collected using the MAR345 imaging plate detector on line X7B. With the shorter surfactant tail, this crystal structure demonstrates the nascent formation of a columnar micelle-type structure similar to that seen for the more zinc chloride rich compositions templated with longer surfactants.

Acknowledgments: NSF DMR-9501370 and DMR-0072828, the Research Corporation, and DOE BES contract DE-AC02-98CH1088

References:

[1]. S. Biggin and J. Enderby, *J. Phys. C: Solid State Phys.*, **14**, 3129, (1981).
[2]. C. L. Keary, T. A. Thornton, M. P. Novotnak, J. D. Martin, Manuscript in preparation
[3]. J. D. Martin and T. A. Thornton, "Liquid Crystal Materials and Devices" Ed. T. J. Bunning, *Proc. Mat. Res. Soc.*, **559**, 243, (1999).

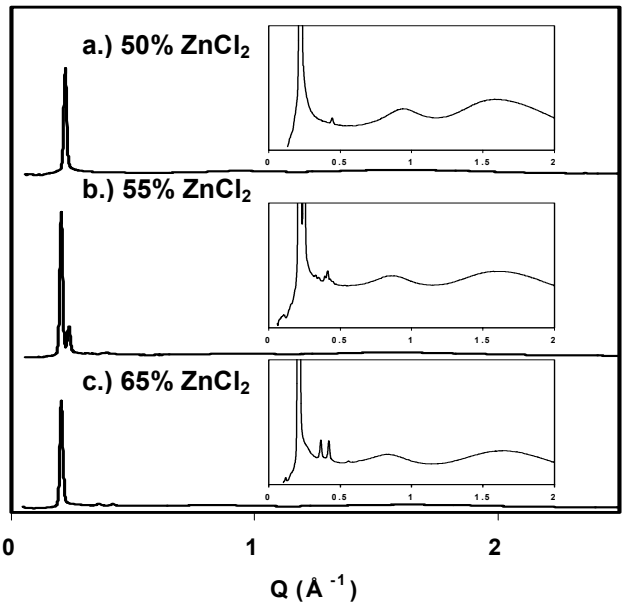

Figure 1. VT-XRD of liquid crystalline phases (a) lamellar (b) cubic (c) hexagonal

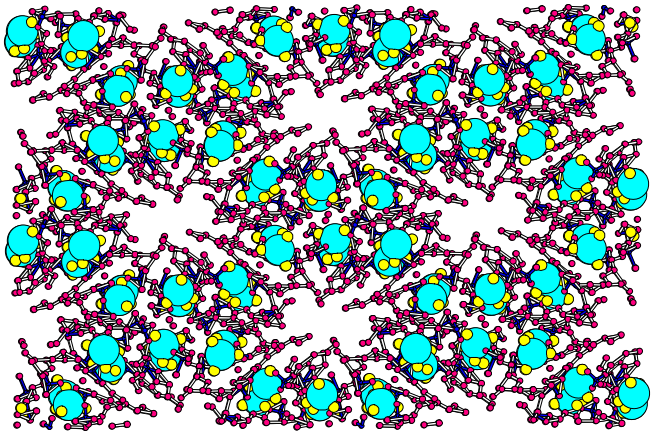

Figure 2. Structure of $[C_8TA]_2ZnCl_4$