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Automation of liquid crystal phase analysis for SAXS

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Lyotropic liquid crystal phases (LCPs) are widely studied for diverse applications, including protein crystallization and drug delivery. The structure and properties of LCPs vary widely depending on composition, temperature and pressure. Therefore, high-throughput structural characterisation, such as small-angle x-ray scattering (SAXS), is important to cover meaningfully large compositional spaces. Currently there are well established methods for high-throughput LCP synthesis using automated methods, and for high throughput SAXS data collection with synchrotron sources. However, high-throughput LCP phase analysis for SAXS data is currently lacking, particularly for patterns containing multiple phases. Using SAXS data, we have developed a high throughput LCP phase identification procedure. The accuracy and time-saving capabilities of the identification procedure were validated on a total of 668 diffraction patterns for the amphiphile hexadecyltrimethylammonium bromide (CTAB), in 53 acidic or basic solvents containing ethylammonium nitrate (EAN) or ethanolammonium nitrate (EtAN). The thermal stability ranges and lattice parameters for the obtained LCP systems showed equivalent accuracy to manual analysis. A time comparison demonstrated that the high throughput phase identification procedure was over 20 times faster than manual analysis. We then applied the high throughput identification procedure to 332 diffraction patterns of sodium dodecyl sulfate (SDS) in the same EAN and EtAN based solvents to produce previously unreported phase diagrams that exhibit phase transitions between hexagonal, lamellar, primitive cubic and diamond cubic LCPs. The accuracy and significant time decrease of the high throughput identification procedure validates a new, unrestricted analytical method for the description of LCP phase transitions.

Level of Expertise

Student

Presenter Gender

Man

Pronouns

He/Him

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

Yes

Do you wish to take part in the Student Poster Slam

Yes

Condition of submission

Yes

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