

Analyses of Porosity and Ability of Guest Accommodation of Columnar Liquid Crystals Derived from a Macrocycle Using Reconstructed Electron Density Maps

(¹Graduate School of Science, Nagoya University, ²NIMS) ○Shin-ichiro Kawano,¹ Masafumi Yoshio,² Takahiro Taki,¹ Kentaro Tanaka¹

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Recently, we reported a shape-persistent macrocycle composed of carbazole and salphen with a 1.4 nm in inner diameter. The macrocycle having branched long side chains exhibits columnar liquid-crystalline (LC) phases over a wide temperature range.¹ However, the existence of substantial nanopore in the LC columnar assemblies has not been elucidated with a direct experimental evidence. In this study, we reconstructed electron density maps (EDMs)² from intensities of the powder X-ray diffraction of the liquid crystal to analyze porosity and ability of guest accommodation of the liquid crystal. An EDM analysis of the liquid crystal suggested that the LC phase consists of two different columns of the stacked macrocycles (Figure A, B) and a low electron density site was revealed in the middle of one of the columns, indicating existence of a discrete nanospace in the columnar liquid crystal. In contrast, an EDM of a liquid crystal accommodating guest molecules shows that higher electron density occupies the nanospace.

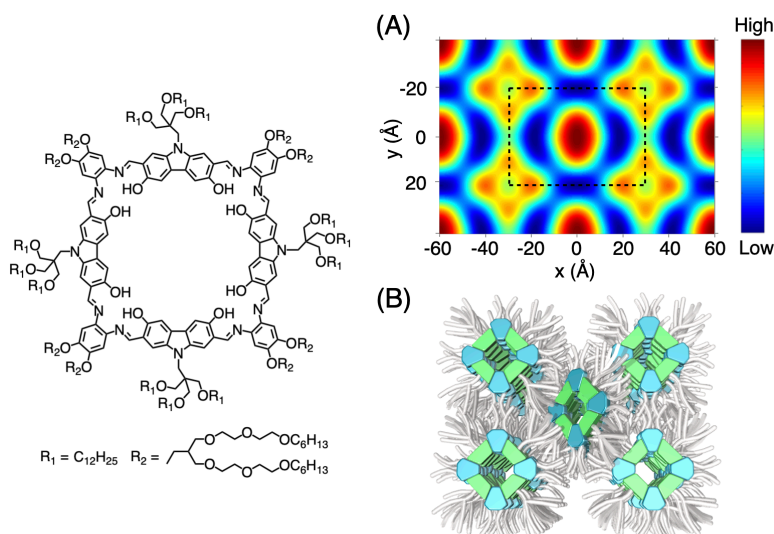


Figure Chemical structure of LC macrocycle. (A) EDM and (B) postulated model structure of the LC phase. Dashed lines in (A) indicate the unit cell.

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