軸不斉をもつナフタミド誘導体のラセミ化合物からコングロメレートへの構造転移

（阪大基礎工[1]・阪大院基礎工[2]）○池田 紗希[1]・桶谷 龍成[2]・久木 一朗[2]
Structural transition behavior of axially chiral naphthamide derivative from racemic compound to conglomerate ([1]*School of Engineering Science, Osaka University*, [2]*Graduate School of Engineering Science, Osaka University*) ○Saki Ikeda,[1] Ryusei Oketani,[2] Ichiro Hisaki[2]

Chiral crystal is a promising material class for applications such as circularly polarized light emission materials and nonlinear optical materials. The purpose of the study is to develop a novel method for preparing chiral crystals through structural transition. Herein, we investigated crystallization and structural transition behavior of axially chiral naphthamide derivative **1**. Powder crystals of the racemic compound underwent a structural transition to conglomerate crystals upon heating, as confirmed by PXRD measurements. The time course of the structural transition was quantitatively analyzed, and the rate constant was calculated based on Avrami plot. The single-crystal-to-single-crystal nature of the transition was characterized using differential interference contrast microscopy and SCXRD.
Keywords：Chirality; Structural transition; Axial chirality; racemic compound; conglomerate

キラル結晶は非線形光学特性などをもつ材料への応用の観点から有望な材料群である。本研究では軸不斉を持つナフタミド誘導体 **1** の結晶の構造転移におけるキラリティ制御を目的とし、化合物の結晶化および構造転移挙動について調べた。粉末 X 線回折測定により、**1** のラセミ化合物の粉末結晶が加熱によってコングロメレート結晶へと構造転移したことを確認した（Figure 2）。異なる温度で構造転移の経時変化を追跡し、Avrami の式に基づいてフィッティングを行い、転移の速度定数を見積もった。さらに、単結晶 X 線構造解析および微分干渉顕微鏡観察から単結晶性を維持した構造転移であることを確認した（Figure 3）。

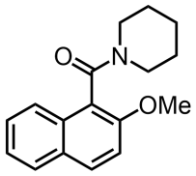

Figure 1. Molecular structure of **1**.

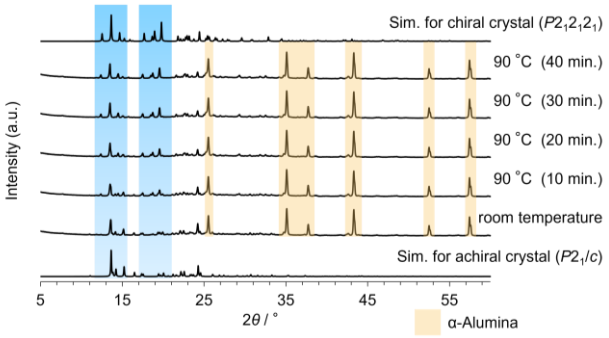

Figure 2. Time course of PXRD patterns for achiral crystals of **1** at 90 °C. α-Alumina was used as internal standard.

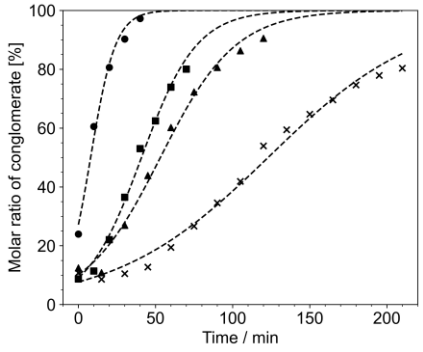

Figure 3. Time course of molar ratio of conglomerate upon the transition at (●) 90 °C, (■) 85 °C, (▲) 80 °C, and (×) 75 °C.