

N-エチル-N'-プロピルジケトピロロピロール誘導体の結晶多形

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Polymorphs of *N*-ethyl-*N'*-propyl-diketopyrrolopyrrole derivative (¹*Graduate School of Environment and Information Sciences, Yokohama National University*) ○Rino Hasegawa¹, Sung-Hoon Kim¹, Shinya Matsumoto¹

Diketopyrrolopyrrole (DPP) dyes had been investigated as a candidate for organic pigments, and chlorinated DPP (PR254) is widely used as a red pigment with good fastness. In a previous study, derivatives of PR254 with a propyl group introduced at both or one of the two amino groups were synthesized and their crystallization were carried out. From both derivatives, crystal polymorphs were successfully obtained, and further dynamic behavior associated with thermal phase transition was observed in their polymorphs. In this study, PR2-3 (Fig. 1 (left)) was synthesized by introducing ethyl and propyl groups into the two amino groups of PR254, and its polymorphism and thermal behavior were investigated. As a result of crystallization, various crystal with different colors and shapes were obtained, and X-ray analysis revealed that the orange and red crystals shown in Fig. 1 are crystal polymorphs. The red crystals were also found to change to orange crystals with dynamic behavior such as jumping when heated.

Keywords : Diketopyrrolopyrrole ; Functional dyes ; Crystal polymorph ; Thermal phase transition

ジケトピロロピロール(DPP)系色素は、有機顔料の候補化合物として検討されており、中でも塩素化 DPP は、堅牢性が良好な赤色顔料(PR254)として広く利用されている。DPP 骨格のアミノ基に置換基を導入すると、溶解度が向上することや、蛍光を示すことが報告されている。先行研究では、PR254 の 2 つのアミノ基の両方あるいは片方にプロピル基を導入した誘導体を合成し結晶化の検討を進めたところ、結晶多形が得られることに加え、一部の多形では、熱相転移に伴う動的挙動が確認された¹⁾²⁾。本研究では、PR254 の二つのアミノ基に、エチル基とプロピル基をそれぞれ導入した PR2-3 (Fig. 1 (left))を合成し、その多形発現や熱挙動の有無を調べた。結晶化の結果、色や形状が異なる様々な結晶性固体が得られ、解析の結果、Fig.1 に示す橙色の結晶と赤色の結晶が結晶多形であることが分かった。また赤い結晶は、加熱をすることにより飛び跳ねなどの動的挙動を伴って橙色の結晶に転移することが分かった。

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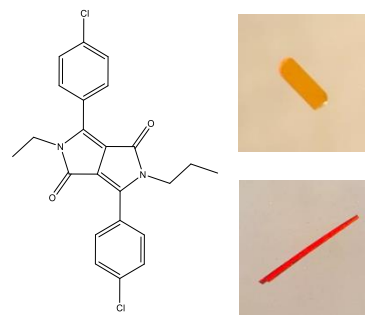


Fig. 1 Molecular structure (left) and obtained two polymorphs (right) of PR2-3.