

N,N'-ジプロピルイソインジゴ誘導体の3つの結晶多形

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Three polymorphs of *N,N'*-dipropylated isoindigo derivative (¹*Graduate School of Environment and Information Sciences, Yokohama National University*) ○Wataru Jozuka,¹ Sung-Hoon Kim,¹ Shinya Matsumoto¹

Alkylation of dye chromophore was known to result in the occurrence of polymorphism in addition to the improvement of solubility.^{1) 2)} In our previous study, *N,N'*-dipropylated isoindigo derivative (Fig 1(a)) was found to have two polymorphs (Forms I and II) with different molecular packing.³⁾ In further crystallization experiments, we obtained its third polymorph (Form III). The molecular structural overly and molecular arrangement of these three forms are also illustrated in Fig 1. Form III has a significantly different molecular conformation and molecular arrangement from those of the other two polymorphs. Different packing arrangements in these three forms was correlated with the difference in the intermolecular interactions. The result of thermal analysis as well as thermally-induced dynamic behavior on these three forms will be also presented.

Keywords : *Isoindigo; Functional dye; Crystal Polymorph; Dynamic behaviour*

色素へのアルキル基導入は、色素の溶解性向上に加え、結晶多形の発現に寄与する場合がある。¹⁾²⁾ これまでの研究で、プロピル基を導入したイソインジゴ誘導体 (Fig 1 (a))から、分子配列の異なる2つの結晶多形 (Form I、Form II) が得られた。³⁾ その後の検討で、3つ目の結晶多形 (Form III) を得ることができた。Fig 1(b)に三つの多形の分子構造を重ね合わせた図を、Fig 1(c)から(e)にそれぞれの多形の分子配列を示す。Form IIIの結晶多形は、2つの結晶多形と比べて、分子配座と分子配列が大きく異なっている。これらの3つの多形の分子配列の違いには、分子間相互作用の違いが大きく影響していることが分かった。本発表では3つの多形の熱分析の結果と、加熱による動的挙動の検討結果も報告する。

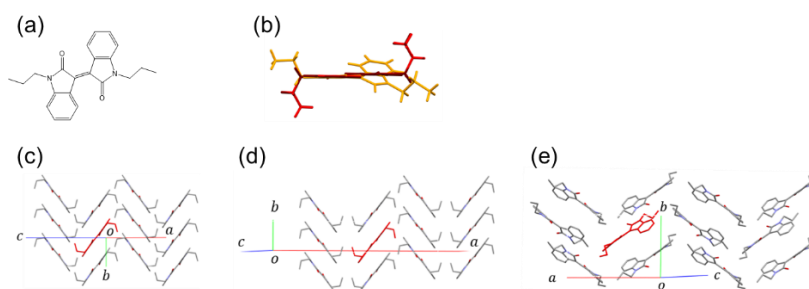


Fig. 1 (a) Chemical structure of the isoindigo derivative, (b) Molecular structural overlay of the three forms in the wireframe style (dark red: Form I, red: Form II, orange: Form III), Molecular arrangement of (c)Form I, (d) Form II, and (e) Form III.

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