N,N'-ジプロピルキナクリドンの結晶多形

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Polymorphs of *N,N'*-dipropylquinacridone ([1]*College of Engineering Science, Yokohama National University*, [2]*Graduate School of Environment and Information Science, Yokohama National University*) ○Yukiko Udo[1], Yugo Suzuki[2], Saori Gontani[2], Shinya Matsumoto[2]

Alkylation of dye chromophore is known to result in the occurrence of polymorphism in addition to the improvement of solubility.[1), 2)] Quinacridone is used as organic pigments as well as a functional dye. Quinacridone and its N-butylated derivative[3)] were reported to have some polymorphs. In this study, we synthesized a quinacridone derivative with propyl groups introduced into its two amino groups (Fig 1(a)). A red polymorph of the present derivative (QA3R) was obtained from an evaporation method, and its orange polymorph (QA3O) from a diffusion method. Deep-red hydrated crystals were also obtained from the same crystallization samples where each polymorphs appeared. QA3O and QA3R had similar 2D layer structures (Fig. 1(b),(c)), but the stacking motif of the 2D layers was different. In QA3R, the molecules stack with alternate slipping along the long molecular axis, while in QA3O, the molecules stack in a staircase fashion. The hydrated crystal was found to have a different packing arrangement characterized by a brickwork structure (Fig 1(d)).

Keywords：Quinacridone; Organic pigment; Functional dye; Crystal Polymorph; Hydrated crystal

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)] 有機顔料や機能性色素として利用されているキナクリドンは、無置換体に加えブチル体[3)]などに複数の多形が報告されている。本研究では、キナクリドンの二つのアミノ基にプロピル基を導入した誘導体(Fig 1(a))を合成した。この化合物について多形探索を行った結果、蒸発法から赤色多形(QA3R)が、拡散法からオレンジ色多形(QA3O)が得られた。また、QA3R や QA3O が得られた結晶化試料から、深赤色の水和結晶も得られた。QA3O と QA3R では、二次元層上の配列は類似だが、その積層の様子が異なっていた(Fig 1(b),(c))。QA3R では、分子が長軸に沿って交互にずれながら積み重なっていたが、QA3O では、分子が階段状に積み重なっていた。水和結晶は二つの多形と異なり、レンガ状の構造を形成していた(Fig 1(d))。

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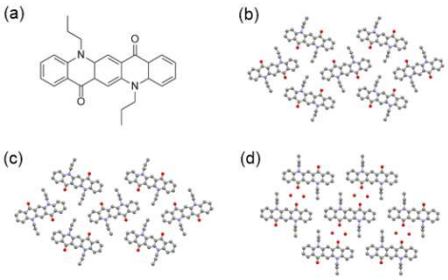

Fig. 1 (a) Chemical structure of *N,N'*-dipropylquinacridone, 2D molecular layer of (b)QA3R, (c) QA3O, and (d) Hydrate.