Polymorphs of two N-alkylated isoindigo dyes

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Isoindigo is a reddish dye having an analogous dye chromophore of indigo which is a traditionally important dyestuff. Isoindigo has been investigated as a functional dye for applications in organic solar cells as well as organic semiconductor [1-3]. N-alkylation of dye chromophore has been known as a usual method to improve its solubility to organic solvents. In addition to this, this modification was reported to result in the occurrence of polymorphism in several dyes [4-6]. In this study, two N-alkylated isoindigo dyes, diethylated derivative 1 and dipropylated derivative 2, were synthesized for tracking their polymorphic forms. We made an attempt to obtain their polymorphs using several crystallization methods with a combination of solvent and temperature. Red-coloured crystals with several different shapes were prepared from 1. X-ray analysis of the prepared crystals revealed that 1 exhibited two polymorphs with same red colour, one is named as the platelet form (1A) and another is the needle form (1B). Molecular conformation and crystal structure of these two forms are shown in Fig. 1. Both planarity of the chromophore and the geometrical relationship of two ethyl groups are significantly different in two polymorphs. Typical herringbone arrangement was recognized in 1A, whereas molecular arrangement of 1B is herringbone-like structure. We also obtained red-coloured crystals of 2 with several different shapes. As a result of their X-ray analysis, 2 was found to exhibit two polymorphs with same red colour, one is named as the platelet form (2A) and another is the needle form (2B). As shown in Fig.2, there is no significant difference in the molecular conformation in these polymorphs, whereas their molecular arrangements are significantly different.

Figure 1. Molecular conformation and molecular arrangement of (a) 1A and (b) 1B.

Figure 2. Molecular conformation and molecular arrangement of (a) 2A and (b) 2B.