Variable Temperature Polymorphism of 2-benzoyl-N,N-diethylbenzamide

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2-Benzoyl-N,N-diethylbenzamide (BDB) was first synthesized as a potential candidate for antispasmodic drugs by Sakamoto et al. (1950) and the thermal profile of the compound was studied by the author (m.p. = 51.1 °C) [1]. The compound was also studied by different research groups where a different value of melting point was reported (m.p. = 76 -77 °C) [2,3]. It is known that different polymorphs can have different physicochemical properties however, the crystal structures of BDB were not elucidated, and assign the correct form of BDB with the melting point was not possible. In 2004 the compound was synthesized by Sakamoto et al. as a precursor for asymmetric synthesis and the crystal structure of an orthorhombic form of BDB was obtained. However, the melting point of this form was not reported by the author [4]. This work aims to assign the melting point with the correct polymorph of BDB and screen for new polymorphs in non-ambient conditions. Here, we identify new phases of BDB using single-crystal x-ray diffraction and variable temperature x-ray powder diffraction and establish the correlation between crystal structure and thermal properties for this compound.

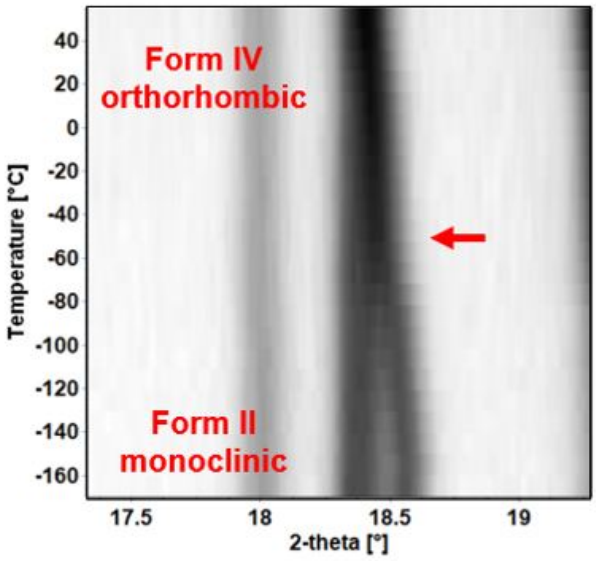

Figure 1