

Poster

Quinolines as optimal Halogen-Bonding acceptors

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Quinolines are molecular species often found in multi-component crystalline systems due to their great ability of participating in intermolecular interactions [1,2], specifically due to the presence of the aromatic nitrogen in the quinolines' core, known as a reliable supramolecular tool [3]. In addition to the pyridinic nitrogen, the quinoline-derivative, quinoline-6-carbonitrile (Q6CN), used in this work, also features a nitrile group that can also act as hydrogen and halogen-bonding acceptor, HB and XB respectively, being possible in this way to understand the competition between supramolecular synthons [4].

From a fundamental point-of-view, the HB and XBs exhibit remarkable similarities: Both are primarily characterized as electrostatic interactions. While in the case of HBs, a hydrogen atom is shared between two electronegative atoms, e.g. oxygen and nitrogen, in the case of XBs the electron-donor species interact with the positive site of halogens, known as σ -hole. Besides the strong electrostatic component, these interactions are also explained by a charge-transfer component when considering the classical Lewis-scheme [5].

To perform this study, the Q6CN molecule was complexed with two different XB donors, 1,4-diiodotetrafluorobenzene (DITFB) and 1-bromo-4-iodobenzene (1B4IB), by mechanochemistry and later crystallized by classical solution methods. The choice of these species was made to evaluate both the competition between the nitrile and pyridine synthons and the influence of fluorination in the XB donors that is known to increase the XB-donor ability due to electronic induction by the fluorine atoms.

The co-crystals were characterized by Single-crystal X-ray diffraction (SC-XRD), Powder X-ray diffraction (PXRD), Differential Scanning Calorimetry (DSC) and Fourier-Transformed Infra-red spectroscopy (FTIR). Based on the calculated wave-functions retrieved from the atomic positions of the crystalline structures, Fig. 1, non-covalent interactions were studied with the NCI and IGM-qg methods [6]. A charge-transfer analysis was also performed by the Natural Bond Orbital method (NBO) [7].

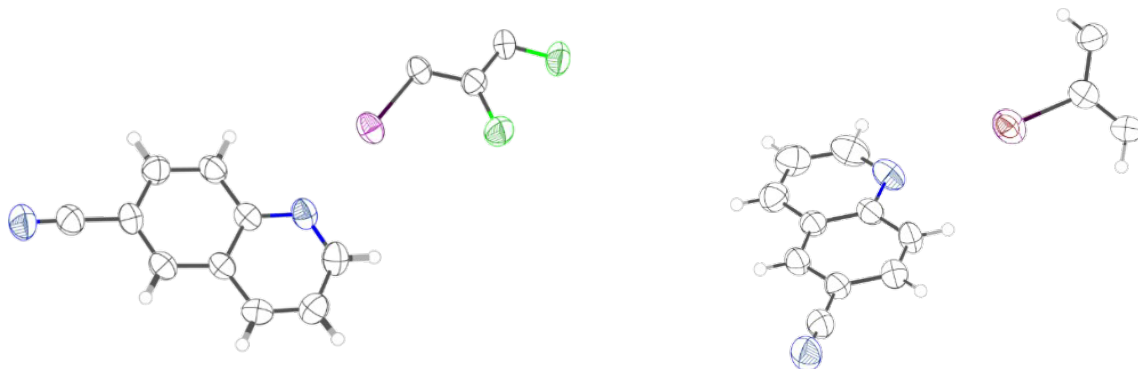


Figure 1. Asymmetric units of the Q6CN-DITFB (left) and Q6CN-1B4IB (right) co-crystals.

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