From Carboxylic Precursors to Thioxanthones: Interplay of Hydrogen Bonds, Br…nitro, S…carbonyl and π…π Stacking Interactions

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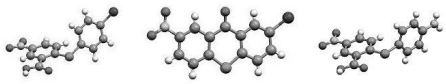
Recently large effort has been set into the synthesis of helical molecular systems, such as sterically overcrowded alkenes. These can be used as photorefractive materials as they allow the presence of measurable dipolar and magnetic contributions to NLO effects[1]. The helical environment is due to the presence of bulky substituents causing sufficient hindrance between the upper and lower half of the alkene to enforce a helical distortion [2].We present here the results obtained in the precursors and thioxanthene used as basic templates. A systematic study of the intra and inter hydrogen bonds and intermolecular interactions is presented, due to its relevance in the folding and packing of the molecules [3].



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