

Title: Evaluation of intermolecular interactions in thioxanthone derivatives: substituent effect on crystal diversity

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Abstract: A family of 9H-thioxanthen-9-one derivatives and two precursors, 2-[(4-bromophenyl) sulfanyl]-5-nitrobenzoic acid and 2-[(4-aminophenyl) sulfanyl]-5-nitrobenzoic acid, were synthesized and studied in order to assess the role of the different substituent groups in determining the supramolecular motifs. From our results we can conclude that Etter's rules are obeyed: whenever present the -COOH head to head strong hydrogen bonding dimer, R-2(2)(8) synthon, prevails as the dominant interaction. As for -NH₂, the best donor when present also follows the expected hierarchy, an NH center dot center dot O(COOH) was formed in the acid precursor (2) and an NH center dot center dot center dot O(C=O) in the thioxanthone (4). The main role played by weaker hydrogen bonds such as CH center dot center dot center dot O, and other intermolecular interactions, pi-pi and Br center dot center dot center dot O, as well as the geometric restraints of packing patterns shows the energetic interplay governing crystal packing. A common feature is the relation between the p-p stacking and the unit cell dimensions. A new synthon notation, R', introduced in this paper, refers to the possibility of accounting for intra- and intermolecular interactions into recognizable and recurring aggregate patterns.

KeyWords Plus: Hydrogen-Bond Patterns; Organic-Compounds; CH/PI Interaction; C-H; Recognition; Complexes; Molecules; Chemistry; Database; Network

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