MS31-2-1 Pseudo and real symmetries for structural optimization of chromeno[4,3-b]quinoline derivatives #MS31-2-1

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Abstract

A novel synthetic method was developed for the construction of chromenoquinoline derivatives from arylpropynyloxy-benzonitriles and diaryliodonium triflates via an oxidative arylation−cyclization path [1]. The method enables the synthesis of chromenoquinoline derivatives with high modularity due to the ease with which variable functional groups can be built into the reaction.

In the presented study the 7-phenyl-6H-chromeno[4,3-b]quinoline is substituted on the phenyl ring at *para* position by a methyl, a methoxy, an acetyl or a carboxymethyl group. The crystal structures have undergone on a gradual modification while the nature of the substituents has been changing (alkyl => ether => ketone => ester) averting the mutual orientation and the point group symmetry of the molecular pairs, as well as the Z value. The effect of the increasing size of the derivatives of the molecules and the increasing number of acceptor atoms on the crystal structures are discussed. None of the derivatives has any classical hydrogen bond donor atom, only C-H...O or C-H...N hydrogen bonds are possible in the structures. However, the 7-phenyl-6H-chromeno[4,3-b]quinolines have an extended hetero-aromatic ring system with potential π... π stacking affinity. The stacking of the molecules is found to be significantly influenced by the electronic effect of the substituents in para position on the phenyl ring. The moderately electron withdrawing groups influence the electron distribution of the aromatic rings in the way that the centrosymmetric stacking of the molecules becomes favourable [2].

References

[1] Klára Aradi, Petra Bombicz, Zoltán Novák: Modular Copper-Catalyzed Synthesis of Chromeno[4,3-b]quinolines with the Utilization of Diaryliodonium Salts *J. Org. Chem*. 2016, 81, 920−931.

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Formulas of the chromenoquinoline derivatives