

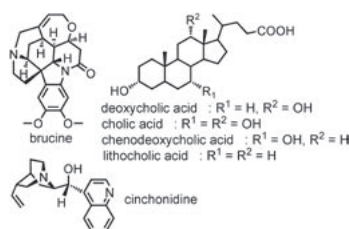
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Supramolecular tilt chirality in crystals of cholic acids

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A concept of supramolecular chirality has assumed increasing importance in association with development of supramolecular chemistry over the last two decades. In chiral crystals, 2[1] helical molecular assemblies are frequently observed as key motifs. Helical handedness of the 2[1] assemblies, however, has not been determined from the mathematical, crystallographical viewpoint. In this context, we have proposed a new concept, tilt chirality. On the basis of the concepts, we describe supramolecular chirality and determine the handedness of 2[1] assemblies composed of relatively complicate molecules with multiple stereogenic centres such as bile acids, brucine, and cinchona alkaloids.



Keywords: alkaloid, helical structure, supramolecular chirality

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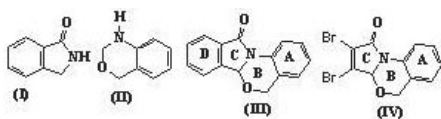
Structure of dihydro-isoindolo benzoxazine-11-one and dibromo-cyclopenta[a]naphthalene-1-one

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Isoindolin-1-one (I) and 2,4-dihydro-1H-benzo[d][1,3]oxazine (II) units are commonly present in synthetic and natural products as simple structures or as a part of complex systems. The syntheses of isoindolin-1-one and 1,3-benzoxazine derivatives have drawn much attention due to the wide range of their biological activities. As part of a continuing study of synthesis of isoindolo-oxazinone and pyrrolo-oxazinone derivatives and we report here the molecular and crystal structures of (III) and (IV). In the molecule of (III), rings D and C are nearly coplanar with dihedral angle of 2.06(4)°. The dihedral angle between A and D rings is 21.22 (3)°. Ring B is not planar and adopts half-chair conformation [1]. In (IV), there are two symmetry-independent molecules in the asymmetric unit and the molecule is not planar, with dihedral angles of 26.5(2)° and 22.1(2)° with A and C, respectively. Ring B is not planar and adopts half-chair conformation.

[1] Boeyens, J. C. A., J. Cryst. Mol. Struct. 1978, 8, 317-320.



Keywords: isoindoline, benzoxazine, fused ring systems

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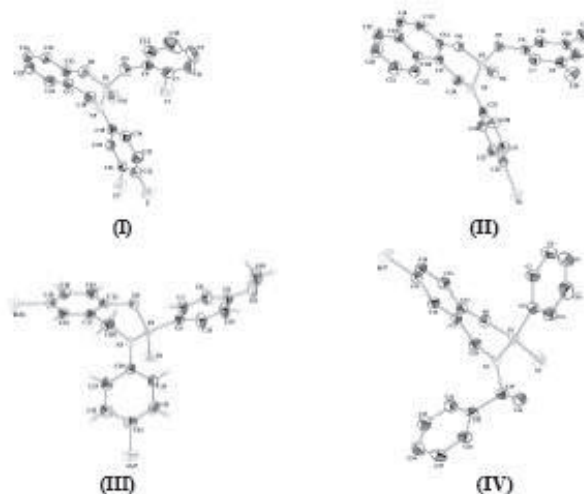
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Effects of substituents on the oxazaphosphorine heterocyclic compounds

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An increasing interest has been sustained in the chemistry of phosphorus heterocycles owing to their unique physicochemical properties and potential biological activities. Many classes of phosphorus heterocyclic system bearing P-O and P-N units, such as cyclophosphamide and its derivatives, are antitumor agents. The title compounds exhibit antifungal activity against *Curvularia lunata*. Because of these activities, the X-ray crystal structures shown below are of great interest to our continuing investigations. A comparison between the structures [II & IV] which differs respectively with substituents of dimethylphenoxy and phenyl at P, shows that the oxazaphosphorine ring assumes a sofa and half-chair conformations. A similar comparison between the compounds [I & III] exhibits a screw-boat for the former and a boat conformation for the later chlorophenoxy and methoxyphenyl as substituents respectively. The analysis on the above four oxazaphosphorine derivatives, suggests that the substituents at P are playing a major role on the conformation of the six-membered heterocyclic ring.



Keywords: organophosphorus compounds, oxazaphosphorine rings, antifungal agents

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Crystal and molecular structure of 4-7-dimethyl,2-H chromen-2-one

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