

zeolites(3); and many have biological applications(4). In this work we report an interesting and unusual non-ambient solid state phase transition of the title compound and postulate a mechanism for how the phase change occurs. We also describe and compare the packing arrangements of both phases as well as the complex intermolecular interactions that occur within the compound itself. The room temperature phase, Form I, is disordered and occupies the space group $P2_1/c$. The low temperature phase, Form II, is perfectly ordered and occupies the space group $P2_1/c$. Differential scanning calorimetry confirms the evidence of both phases of the title compound.

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Keywords: low-temperature crystallography, differential scanning calorimetry, n-alkyl-diammonium salts

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Synthon polymorphism in dihydroxybenzoic acids

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Polymorphism, the existence of more than one crystalline modifications of the same compound, has great importance in pharmaceuticals, agrochemicals, pigments, dyes and explosives. Polymorphs have different physical and chemical properties, such as melting point, density, compressibility, solubility, hardness, dipole moment and bioavailability. Multifunctional molecules are capable of making different supramolecular synthons in different crystal structures, or synthon polymorphs. Sublimation and melt crystallization were shown to give guest free forms through a green methodology.¹ These techniques are now employed to generate new polymorphs of 2,3-, 2,4-, 2,5-, 2,6-, 3,4-, and 3,5-positional isomers of dihydroxybenzoic acids. These compounds are prone to give solvate/hydrate forms upon crystallization. Two polymorphs of 3,5-dihydroxybenzoic acid, a new polymorph of 2,3-dihydroxybenzoic acid and guest free form of 3,4-dihydroxybenzoic acid were crystallized by melting and sublimation. A new hydrate polymorph of 3,4-dihydroxybenzoic acid was isolated. These polymorphs differ in the nature of hydrogen bond synthons in their crystal structure. Structural and thermal characterization of polymorphic phases having multiple Z' will be presented.

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Keywords: polymorphism, inclusion compounds polymorphism, organic crystal structures

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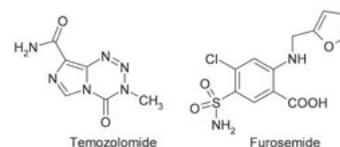
Conformational polymorphs of temozolomide and furosemide

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The pharmaceutical industry is frequently confronted with the phenomenon of multiple crystal forms of the same chemical entity. Two Active Pharmaceutical Ingredients (API), Temozolomide (TMZ) and Furosemide (FUR) are chosen to study the influence of conformer changes on hydrogen bonding and crystal packing. Apart from a known crystal structure of TMZ form 1, two new crystalline modifications, form 2 and 3, were obtained during attempted co-crystallization with carbamazepine and 3-hydroxypyridine-N-oxide. Conformers A and B of TMZ are stabilized by intramolecular hydrogen bonds with imidazole and tetrazine N atoms. The stable conformer A is present in TMZ polymorphs 1 and 2 whereas both conformers crystallized in TMZ form 3. Similarly three polymorphs of FUR are characterized. High energy conformers (4.49 kcal/mol) are present in stable FUR form 1 while a stable conformer is present in the metastable FUR 2 and 3 crystal structures. Polymorphism in both these systems is based on differences in conformations and hydrogen bond synthons.



Keywords: drug polymorphism, conformational polymorphism, X-ray characterization of single crystals

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Crystal structures and pseudo polymorphism of anionic surfactants

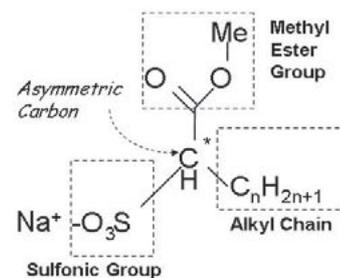
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Crystal structures of anionic surfactants, methyl 2-sulfoalkanoate sodium salts (MSA) in Fig. have been analyzed by X-ray. These types of surfactants are called as methyl ester sulfonate (MES) notably used for commodity detergent as the view point of eco-friendly materials derived from vegetable oil and less emission of carbon dioxide. The determined crystal structures of surfactants are very rare because of the difficulty of the formation of single crystals. The crystals of MSAs show pseudo polymorphism with several hydrated numbers. A hydrated type of crystals transformed to other type of those by the humidity and the hydrated number affects the physicochemical properties of MSAs. Crystals of MSA showed 4 types of hydrate number of anhydrate, two, six, and ten in previous report, 1). The crystal structure of dihydrate (*Pbcm*) has been determined by X-ray in 2). New crystal structures with several hydrate salts of MSAs of racemic crystals have been determined. The single crystals were obtained from aqueous ethanol.

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Keywords: surfactants, detergents, hydrates