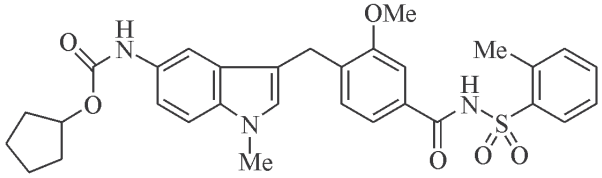
s13.m42.p7 **Molecular Structures of the Zafirlukast Derivatives.** Botoshansky M.[a], Goldring D.[a], Khalfin R.[b], Pertsikov B.[c], Kaftory M.[a], Nisnevitch G.[c], Ponomarev V.[c], Zaltzman I.[c], Gutman A.[c], [a]*Chemistry Department, Technion, Israel,* [b]*Chemical Engineering Department, Technion, Israel,* [c]*Fine Tech Laboratories Ltd, Israel. E-mail: botoshan@tx.technion.ac.il*

Keywords: Zarfirlukast; Derivative; Structure

Zafirlukast (ZAK)- [4-(5-cyclopentyloxy-carbonylamino-1-methyl-indol-3-ylmethyl)-3-methoxy-N-*o*-tolylsulffonyl-benzamide] is well known [1] active part of the drugs for



effective prophylactic treatment of asthma with prolongated affect after drug administration. Different phases and derivatives of ZAK have been founded to possess biological activities. In pursuit possible useful intermediate product for fabrication processes three new polymorphs - zafirlukast monohydrate (I), zafirlukast methanolate (II) and zafirlukast ethanolate (III) have been synthesized and studied by X-ray and thermal analysis. All polymorphs belong to monoclinic symmetry with centrosymmetric space group $P2_1/n$ for (I) and non-centrosymmetric space group *Cc* for (II) and (III). The molecules of ZAK are naturally very similar to each other, but occurrence of different solvent molecules included in crystal structures leads to formation of different hydrogen bond network. There are different molecular packing and different thermal behavior for three polymorphs.

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s13.m42.p8 **The Crystal Structures of the Benzoate, Fumarate and Maleate Salts of 2-Aminopyridine.** Orhan Büyükgüngör[a] and Mustafa Odabasoglu[b], [a]*Department of Physics, Ondokuz Mayis University, TR-55139, Samsun, Turkey, and* [b]*Department of Chemistry, Ondokuz Mayis University, TR-55139, Samsun, Turkey. E-mail: orhanb@omu.edu.tr*

Keywords: 2-Aminopyridine; Benzoic, fumaric and maleic acid; Amino-imino tautomerization

Hydrogen bonding plays a key role in molecular recognition and crystal engineering research. The design of highly specific solid-state structures is of considerable significance in organic chemistry, due to their important applications in the development of new optical, magnetic and electronic systems [1]. Our investigation of the title compounds shows that the 2-aminopyridinium ions are linked to the carboxylate ions through N1-H...O and N2-H1...O hydrogen bonds, resulting in the formation of cyclic eight-membered hydrogen bonded rings (Fig. 1).

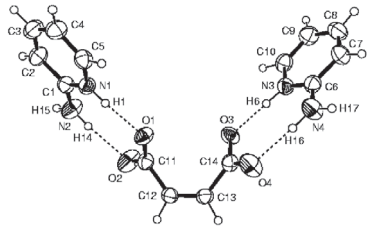

Fig.1. A view of the moieties of bis(2-aminopyridinium) maleate [symmetry code: (i) ½-x, ½-y, z].

Each amino H atom in compounds is involved in a single hydrogen bond, one in the cyclic eight-membered hydrogen-bonded ring system and the other to another carboxylate ion. 2-aminopyridine, like other organic bases, is protonated in acidic solutions. The bonding of the H atom to the ring N atom of 2-aminopyridine, but not to the amino N atom, gives an ion. The C-N-C angle of pyridines is very sensitive to protonation[2]. Due to the complete protonation of the heterocycle in 2-aminopyridinium carboxylates, the C1-N1-C5 angle is enlarged. The 2-aminopyridine-carboxylate system has the amino-imino tautomerization. The main features of amino-imino tautomerization are demonstrated in the structure of the title compounds by the bond lengths and angles of the heterocycle and the carboxylate anions, respectively. Our investigation clearly shows that the positive charge is on the nitrogen atom of pyridine ring[3,4].

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