

Poster Presentation

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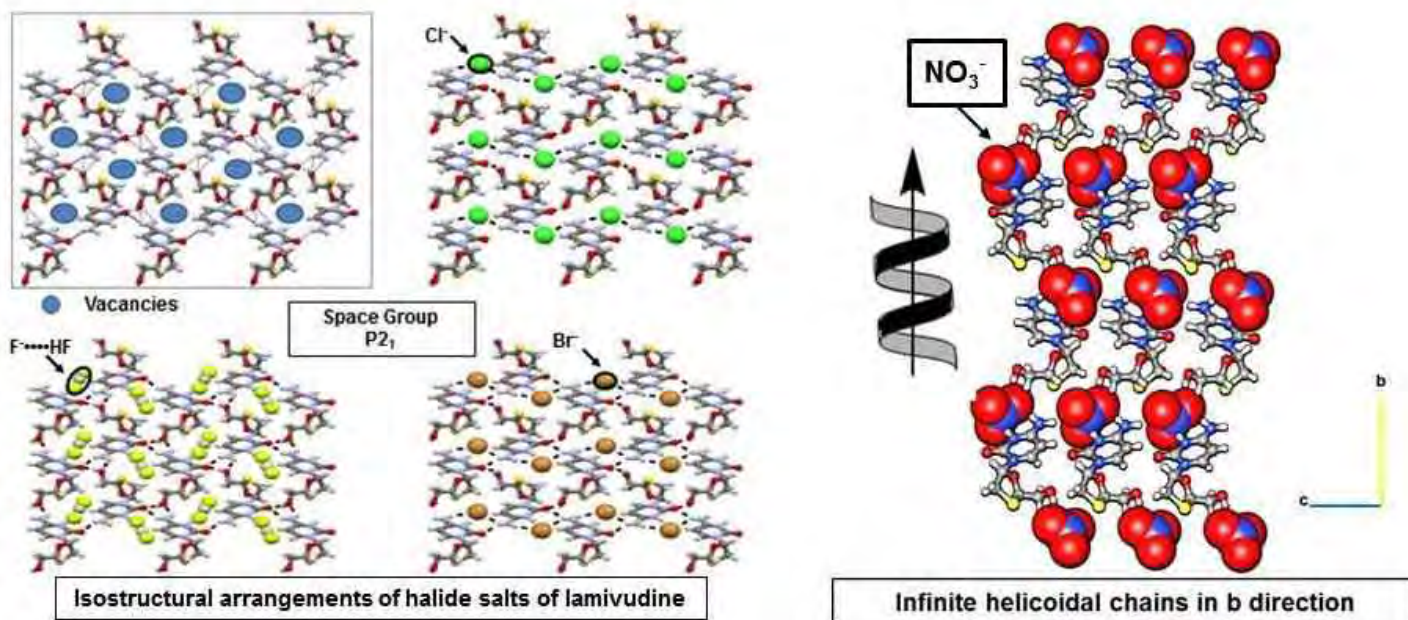
Molecular architectures of new inorganic lamivudine salts, an anti-HIV drug.

J. Tenorio¹, J. Ellena¹

¹Universidade de São Paulo, Instituto de Física de São Carlos, São Carlos/SP, Brazil

One of the currently goals of the crystal engineering is the improvement of pharmaceutical properties of Active Pharmaceutical Ingredients. Herein is discussed the design of new solid forms of the Lamivudine (3TC), one of the most used and marketed anti-HIV drug. The crystalline forms herein presented correspond to inorganic acid salts: Lamivudine hydrobromide ($3TCH^+Br^-$), hydrogen difluoride ($3TCH^+F^-HF$) and nitrate ($3TCH^+NO_3^-$). These new salts crystallized in non-centrosymmetric space group $P2_1$. The halogenated salts ($3TCH^+Br^-$ and $3TCH^+F^-HF$) exhibited isostructural supramolecular assemblies, similar to the anhydrous salt of lamivudine hydrochloride ($3TCH^+Cl^-$) reported by our research group, and whose equilibrium solubility showed an increase when compared with 3TC pharmaceutical form. [1,2] The main feature of the salt crystalline assemblies is related to the supramolecular ordering of the $3TCH^+$ cationic units, by observing the formation of vacancies between them generated in the [100] direction due to the helical symmetry, so, the anions are localized into the interstices of these vacancies, stabilizing the crystalline assemblies. Meanwhile, the $3TCH^+NO_3^-$ salt showed a different conformational and supramolecular behavior from that observed in the halogenated ones. Here is observed the formation of helical strands along the b axis, which will be engaging by translational symmetry in the horizontal direction in the [10-1] plane. Therefore, they form zigzag molecular planes which will subsequently be architected in parallel with the [10-1] direction. In addition, it was used for this study X-ray powder diffraction (XRPD), vibrational analysis: Infrared (IR) and Raman spectroscopy, and thermal analysis: differential scanning calorimetry (DSC), thermogravimetry (TG) and hot-stage microscopy. Comparison of the structural properties of these salts with some forms already reported (e.g. $3TCH^+Cl^-$) allows to infer some possible pharmaceutical properties.

[1] J. Ellena, N. Papararidis, F.T. Martins, *CrystEngComm*, 2012, 14, 2373-2376, [2] F.T. Martins, R. Bonfili, M.B. De Araújo, J. Ellena, *Journal of Pharmaceutical Science*, 2012, 101, 2143-2154



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