Concept of Crystal engineering primarily involves in designing new crystals by understanding the molecular interactions between the components forming the crystal complex.

4-Aminopyridine a heterocyclic compound has been used in the treatment of multiple sclerosis it has also been used to synthesize metal complexes having non-linear optical properties. It can also be used as model compound to understand nucleic acid bases. Complexes of 4-aminopyridine with dicarboxylic acid generally self assemble forming N-H...O and O-H...O hydrogen bonds resulting in supramolecular heterosynthons.

Complex of 4-aminopyridine with dicarboxylic acids in various stoichiometric ratio have been reported. We tried to grow crystals of 4-aminopyrine with maleic acid in 2:1 ratio, as the other stoichiometric ratios i.e 4-aminopyridine maleate [1] and 4-Aminopyridinium-hydrogen maleate-maleic acid [2], had been already studied. Interestingly the crystal obtained was a salt, 4-aminopyridinium 3-(4-aminopyridinium) succinate tetra hydrate. The maleic acid had undergone hydrogenation reaction and converted to succinic acid, and the succinic acid had combine with 4-aminopyridine to form the compound 3-(4-aminopyridinium) succinate. The room and low temperature data were collected on a Bruker-SMART Apex II 4K CCD diffractometer using Mo-Kα graphite-monochromated radiation (λ=0.71073 Å). The Final R indices R[F2 > 2σ(F2)]: 0.042 and 0.044 for room temperature and at 100K respectively. The salt crystallized in noncentrosymmetric space group of P21 21 21 with following cell parameters a=4.8872(1) Å, b=10.5776(2) Å, c=35.3990(6) Å, α=90°, β=90°, γ=90° and Volume: 1829.95 Å³. A comparison of cell parameters at two temperatures shows that the change in cell parameters are, Δa=0.0781Å, Δb=0.0519 Å, Δc=0.0627 Å. The decrease in volume as we go to 100K is 34.91Å³. It seen that the maximum change occurs along a axis followed by c axis. The reduction in temperature brings about closer packing of molecules and general shrinkage of the unit cell to the extent of 2-3%. There is no structural transition in this temperature range. The structure composed of a molecule of 4-aminopyridylne in the protonated state, a 3(4 aminopyridinium) succinate and four water molecules. These molecules are held by N-H...O and O-H...O hydrogen bonds forming a three dimensional network along all the three principal axes. A database search revealed that complexs of 2-aminopyridine with succinic acid has already been reported from 4-aminopyridine and succinic acid in 1:1 and 2:1 ratio, but the salt formation from maleic acid to succinic acid is one of its kind. Apart from this, complextaion of aminopyridine with maleic acid always resulted in a complex of 4-aminopyridine and maleic acid in 1:1 and 2:1 ratio. The detailed structure and a database study of 4-aminopyridine complexes will be discussed.


Keywords: structure, 4-Aminopyridine, maleic acid