**Crystal Engineering of Co-crystal of Nicotinic acid and Pyrogallol: An Experimental and theoretical Electron density Analysis**

Alia Iqbala, Arshad Mehmoodb, Sajida Noureena, \*, Claude Lecomtec,d, Maqsood Ahmeda\*

aMaterials Chemistry Laboratory, Institute of Chemistry, The Islamia University of Bahawalpur, Baghdad-ul-Jadeed Campus 63100, Pakistan.

and bDepartment of Chemistry and Biochemistry, Texas Christian University, Fort Worth, Texas

76129, USA.

c Université de Lorraine; Laboratoire CRM2, UMR CNRS 7036, Boulevard des aiguillettes BP70239, Vandoeuvre-les-Nancy, 54506, France
d  CNRS, Laboratoire CRM2, UMR CNRS 7036, Boulevard des aiguillettes BP70239, Vandoeure-les-Nancy, 54506, France.

Experimental electron density analysis by means of high resolution X-ray diffraction data up to sinθ/λmax=1.11Å-1 at 100(1) K has been performed to analyze the detailed structure and the strength of intermolecular interactions responsible for the formation of a new solid form of Nicotinic acid (**NA**), cocrystallized with Pyrogallol (**PY**) with two NA-PY units in the asymetyric unit. The refinement were carried out using the Hansen and Coppens multipolar formalism (program Mopro). The **2:2** cocrystal of NAPY exhibits a zig-zag, brick stone and sheet like layered structure along 3D and is stabilized by strong intra and inter-molecular hydrogen bonding through N­-H‧‧‧O and O-H‧‧‧O bonds, some of them due to the zwitterion nature of NA as well as weak interactions between the PY molecules. Ranking these interactions via topological analysis of the electron density shows the leading role of the NA···NA sublattice which drives the cocrystals organization. These strong interactions between the NA zwitterions may explain why Z’=2 and why the NA substructure has a larger symmetry than that of the cocrystals .