Poster Presentation

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Hydrogen Bonded Charge Transfer Complex of Chloranilic Acid With Benzimidazole

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The crystal structure of 1:1:1 complex of chloranilic acid with benzimidazole and water determined by X-ray diffraction methods is reported. It crystallizes in the monoclinic (space group, P21/c) crystal system. Both chloranilic acid and benzimidazole molecules adopt a face-to-face stacking arrangement along the b-axis. An interaction beween adjacent layers is a π…π stacking interactions between chloranilic acid molecules. The dihedral angle between the interacting chloranilic acid ring planes is only 1.22 (7)° with an interplanar spacing between C10…C12 (3.383 (16) Å) and C13…C15 (3.351 (14) Å). Water influences proton transfer in the hydrogen bonded charge transfer complex, and contributes to generating increased number of hydrogen bonds utilized in the stabilzaation of the crystal structure of the complex. Water serves as an efficient bridge between the chloranilic acid molecules through O-H…O intermolecular hydrogen bonds to form a zigzag channel, as well as directly linking chloranilic acid molecules with benzimidazole molecules which are strongly entrapped within the zigzag channel by intermolecular hydrogen bonding network involving the N-H…O, C-H…O, and C-H…Cl interactions. In the chloranilate anion structure, an intramolecular hydrogen bonding involving O2-H7 and O1 (dO2… O1 and dH7… O1 = 2.670 (12) and 2.25 Å) occurs. The supramolecular architecture of the hydrogen bonded charge complex exhibits a three-dimensional hydrogen bonding network

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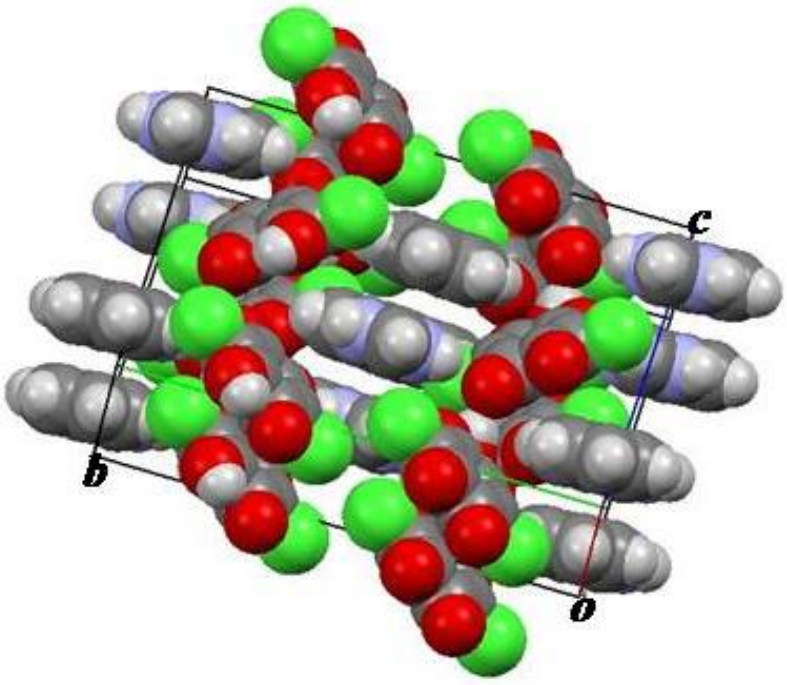

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