Syntheses, Crystal Structures And Hirshfeld Surface Analysis Of Three Salts Of 1-(4-Nitrophenyl)Piperazine

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The structures and Hirshfeld surface analysis of three salts of 1-(4-nitrophenyl)- piperazine are discussed. In 4-(4-nitrophenyl)piperazin-1-ium salicylate there are strong hydrogen bonds between cation and anion and the 4-nitrophenyl substituent occupies an equatorial position in the piperazinium ring. The cation and anion are linked together by supramolecular interactions. Additionally, there is pi-pi stackinginvolving the salicylate anion and the piperazinium cation in adjacent asymmetric units as well as an interaction between a hydrogen atom on the piperazine ring and the phenyl ring within the salicyclate anion. In bis[4-(4-nitrophenyl)piperazin-1-ium] bis(4-fluorobenzoate) trihydrate there are two cations, two anions, and three water molecules of solvation in the asymmetric unit, all linked by hydrogen bonds In the anion, the 4-nitrophenyl ring occupies an axial substitution position in the piperazinium ring, which is relatively rare. In 4-(4-nitrophenyl)piperazin-1-ium 3,5-dinitrobenzoate the 4-nitrophenyl ring occupies an axial substitution position in the piperazinium ring, as seen in the previous structure. In the crystal, the cation and the anion form a complex three dimensional hydrogen-bonded array The nitrophenyl group is disordered with occupancies of 0.806 (10) and 0.194 (10).