Oral Contributions

[MS29 - 02] Charge Density Studies of Nitroimidazoles: Halogen Bonding and Solid Solution. Maciej Kubicki[a], Agnieszka Poulain[a,b,c], Claude Lecomte[b].

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The results of deformation density analysis for three 4-nitroimidazole derivatives: 2-chloro-1¬methyl-4-nitro-1H-imidazole (1), 1-(4¬chlorophenyl)-5-methyl-4-nitroimidazole) (2) and (1-(4'-chlorophenyl)-2-methyl-4-nitro-1H-imidazole-5-carbonitrile (3) will be presented and compared with the previously reported data [1-3]. Multipolar Hansen-Coppens model [4] was applied for the structure refinement, the analysis of the both intra-and intermolecular interactions was mainly performed within the framework of Bader's Atoms¬In-Molecules theory [5]. Compound 1 crystallizes in the Pnma space group and the whole molecule, except two symmetry-related hydrogen atoms of the methyl group, is located on the mirror plane of symmetry. The main packing forces have been identified as halogen and weak hydrogen bonds, and additionally π···π interactions. For 2 relatively strong C-H···O/N hydrogen bonds, π stacking and C-Cl···O directional non-bifurcated halogen bond have been found in the crystal structure, while for 3 the main interactions are weak C-H···O/N hydrogen bonds, dipolar C≡N···C≡N, π stacking and C-Cl···O/Cl halogen bonds. Topological features of these interactions have been analyzed and some correlations between geometrical, topological and energetical characteristics have been found. Crystals of 3 turned out to be a solid solution between the 5-cyano derivative, and one of the substrates, namely 5-bromo compound: presented.

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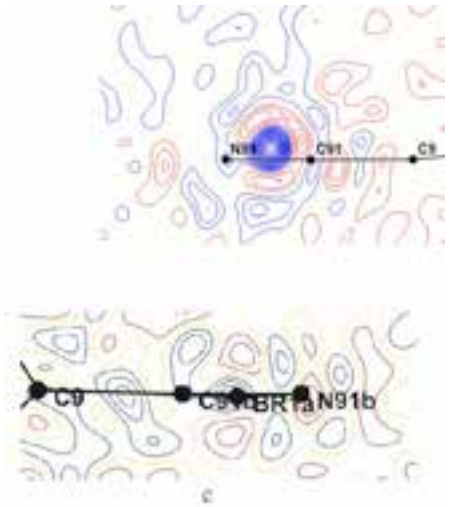

The residual density maps before(top) and after (bottom) incorporating disorder into the model

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