the mutation prevents the protonated N1 nitrogen atom of the PLP pyridine ring from creating a hydrogen-bond with the side chain of residue 214. Instead, new hydrogen bonds are formed between the PLP O3' atom and the side chains of Asn185 and Thr216, and between the deprotonated PLP N1 atom and a nearby water molecule that is hydrogen bonded with Glu103 and Thr126. These new interactions cause a significant conformational change in the active site, including reorientation of PLP and the side chains of Asn185 and Thr103, and translocation of the helix α4', together with the catalytically important Thr124, by ~1.5 Å from the active site cleft. The open active site cleft as a whole is slightly more closed than in the wild type holoenzyme. These results explain the observed inactivity of D214A mutant [5].

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Keywords: vitamin B6, enzymatic structure-activity relationships, mutations

FA4-MS36-P04

Experimental charge density studies, electrostatic and topological analysis of 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole crystals.

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High resolution diffraction data of crystals of small organic molecules, such as 4-nitro-1H-imidazole derivatives, are achievable within a period of days, thanks to the development of the measurement devices.
Processing these data in the standard manner to solve and refine the structures and to obtain the information about the geometry and interactions is usually performed applying the Independent Atom Model (IAM). Within this approximation all atoms are treated as 'spherical balls' with the electron density concentrated around the nuclei. However, this assumption neglects transfer of the charge density into the bonding regions – especially for the covalent bonds – and the transfer associated with the intermolecular interactions.
To improve the electron density distribution model and to allow for the detailed analysis of the intra- and interactions in the molecules and in the supramolecular assemblies, such as the 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole, the Hansen-Coppens formalism [1] and Atoms-in-Molecule approach [2] for topological analysis are used. The multipole model has been implemented in the MoPro program suite [3] and allows electrostatic and topological calculations for both small molecules and biological macromolecules at subatomic resolution.
Within this poster the experimental charge density distribution of the title compound will be presented. The crystal structure of this 4-nitroimidazole derivative was published recently, using standard resolution data [4], however no detailed analysis of the influence of the substituents on the electron distribution was performed. The main observed interactions are the strong and weak hydrogen bonds (N-H···N, N-H···O and C-H···O, C-H···Cg (centroid of the aromatic ring), respectively). These regions, with a special attention paid to the nitro group (as hydrogen bond acceptor), will be analysed.
This is a part of our project to investigate the weak interactions in the series of 4-nitro-1H-imidazole derivatives, to examine the influence of the different substituent groups on the charge density distribution within the aromatic ring.

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Keywords: 4-nitro-1H-imidazole derivatives, multipole refinement, high resolution diffractiondichalcogenides compound, Trigonal prism

FA4-MS36-P05

Supramolecular π-π and Hydrogen Bond Interactions in Arylsulfonate Complexes.

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Six novel compounds were synthesized under hydrothermal conditions by reaction of divalent cations (M^{2+} = Co^{2+}, Ni^{2+}, Mn^{2+}, Cu^{2+} and Zn^{2+}) with two different arylsulfonates and phenanthroline. $Co_2(2,6\text{-AQDS})_2(phen)_4$ (**1**) (2,6-AQDS = anthraquinone-2,6-disulfonate, phen = 1,10-phenantroline) crystallizes in a space group P-1, is a dimeric molecular complex and exhibits 2D supramolecular arragement via π-π aromatic slipped and T-shaped stacking interactions [1]. The compounds $Co(1,5\text{-AQDS})(Phen)_2(H_2O)$ (**2**), $Ni(1,5\text{-AQDS})(Phen)_2(H_2O)$ (**3**), $Mn(1,5\text{-AQDS})(Phen)_2(H_2O)$ (**4**), $Cu(1,5\text{-AQDS})(Phen)_2(H_2O)$ (**5**) and $Zn(1,5\text{-AQDS})(Phen)_2(H_2O)$ (**6**) (1,5-AQDS = anthraquinone-1,5-disulfonate) are a series of isostructural molecular compounds of space group P-1. Their structures are formed by one arylsulfonate and two phenanthroline molecules in octahedral arrangement around the metal cation. These molecular complexes have 2D supramolecular structure by combination of π-π aromatic slipped interaction, T-shaped stacking interactions, as well as C-H…O and O-H…O interactions. Catalytic activity of **1-5** for oxidation of organic sulfides [2] was studied.

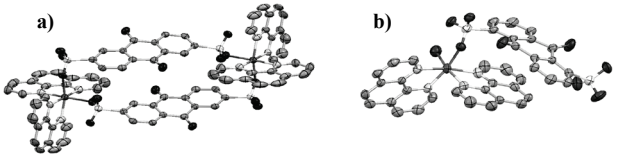

Figure 1. a) Dimeric structure of compound **1** and b) monomeric structure of compound **2.**

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Keywords: Arylsulfonates, stacking interaction, hydrothermal