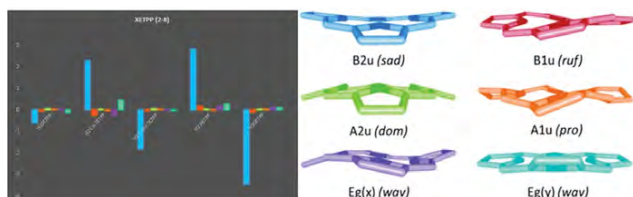


sations. This is mainly seen in the difference between *sad*, *ruf* and *dom* distortions in XETPPs and XETPCs. From the results obtained in this test case, we can now go on and use these observations to discuss the macrocycle conformations in chlorophyll.



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Keywords: NSD, chlorophyll, porphyrins

MS32-P02

Crystal structure investigation for series of salts of 2me-5na with different acids

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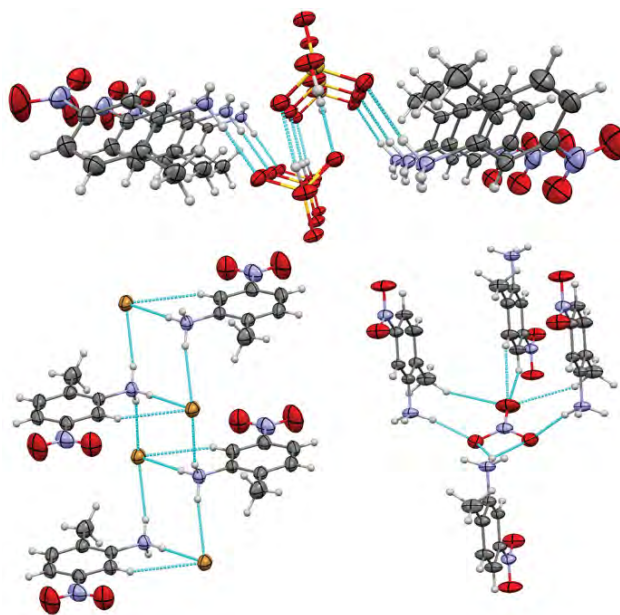
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The many of nitroaniline derivatives are materials with nonlinear optical (NLO) properties [1]. The molecules of nitroanilines contain the amino group which can be protonated and new compounds can be obtained in acidic conditions. Therefore, a search of compounds with NLO properties can be expanded for a large group of organic ionic compounds. Previously, some complexes of 2-methyl-4-nitroaniline with inorganic acids were studied [2]. As a continuation of those studies, here we present crystal structure of six new salts of 2-methyl-5-nitroaniline (2Me-5NA) with inorganic acids.

Five of obtained crystals have centrosymmetric space groups, but one does not have the centre of symmetry. Structures of all the compounds are stabilized by N–H...A⁻ hydrogen bonds between -NH₃⁺ group and inorganic anion. The stability of all the salts was checked in the range 295–100K and no phase transitions were revealed.

Fig. 1. The networks of hydrogen bonds in crystal structures of (H-2Me-5NA)HSO₄, (H-2Me-5NA)Br and (H-2Me-5NA)NO₃ at 295K..



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Keywords: Nitroanilines, NLO, structure