

## MS32-P09 | NON-COVALENT BONDING IN ORGANIC CRYSTALS: A COMBINED X-RAY AND DFT STUDY

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The study of non-covalent interactions is an actual problem for both chemists and biologists, materials scientists, physicists and pharmacologists. Such interest is explained by an important role of non-covalent interactions both in the formation of structures of compounds and in biological, biochemical processes, processes of molecular recognition and self-assembly. One of the most relevant areas today is the search and study of structure – property correlations the identification of which allows us to significantly expand our understanding of the flow of various processes and to regulate them. The most widely studied and described non-covalent interactions are of course the hydrogen bonds, however, interest in weaker and much less studied interactions has recently increased.

In this work, using high-resolution X-ray diffraction analysis and DFT calculations performed for a series of crystals of biologically active organic molecules, we analyzed weak non-covalent interactions such as H-bonds, stacking interactions and Lp..pi (cyclic and non-cyclic) one. Their effect on the electronic, molecular and crystal structure of studied compounds, as well as the propensity of related compounds to form certain non-covalent interactions, is discussed in details. Obtained results are important from the fundamental point of view and as a contribution to crystal engineering concept.

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