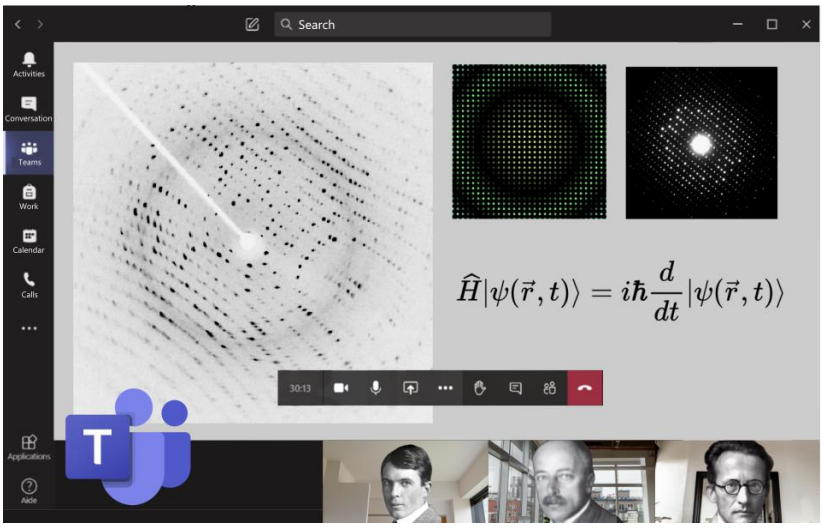
Quantum Crystallography Online Meeting 2020

QCrOM2020



Book of Abstracts

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Fluorination as a Driving Force in Crystal Structures

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The results of the crystallographic analysis in combination with quantum chemical calculations have shown that fluorination of organic compounds causes an increase in the proton-donating ability and a decrease in the proton-accepting capacity of the groups in their neighbourhood[1]. The establishment of F···F interactions causes the electron density to shift towards the area of F···F contact, thus creating a new region with a higher negative potential and the more pronounced accepting ability. This new region has a larger surface area and it is able to form simultaneous interactions with species from the crystal environment. This compensates the reduction of the accepting capacity of the groups in the neigbourhood of the interacting F atoms. Taking into account the formation of this new region, not only the abundance of F···F interactions in the crystal structures (the second largest group of interactions), but also a large number of structures with F···O interactions (third largest group of interactions) can be explained. Only the C–H···F interactions are more numerous than F···F interactions, indicating an increased affinity of fluorinated compounds for non-polar groups.

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[1] G.V. Janjić, S.T. Jelić, N.P. Trišović, D.M. Popović, I.S. Đorđević, M.K. Milčić, Cryst. Growth Des. 2020, 20, 5, 2943–2951.