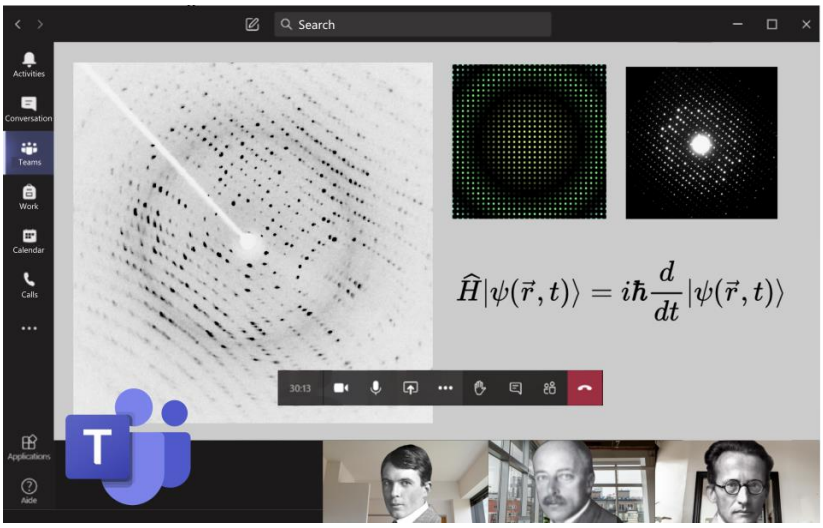
Quantum Crystallography Online Meeting 2020

QCrOM2020



Book of Abstracts

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Substitution of S by Se. Supramolecular Insight.

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Keywords: Substitution of S by Se; Supramolecular structure

The study includes the crystallographic analysis of interactions of S and Se from Cys, Met, Sec and Mse side chains, based on crystal structures from the Cambridge Structural Database (CSD), and quantum-chemical insight in the strength of their individual interactions.
CSD statistical analyses have shown a similar tendency of sulfur and selenium atoms towards the specified types of interactions. The most numerous are C−H···Se (for Se fragments) and C−H···S (for S fragments) interactions (~80%), while the second group in numerosity are structures with Se···Se and S···S interactions (~5%). The results of quantum-chemical calculations have revealed that C−H···S and C−H···Se interactions (about −0.8 kcal/mol) are weaker than the most stable parallel Se/Se interaction (about −3.3 kcal/mol) and electrostatic Se/Se interaction of σ/π type (around −2.6 kcal/mol). The numerosity of C−H···S and C−H···Se interactions was explained by an abundance of CH groups compared to the numbers of Se and S atoms in the analyzed crystal structures. The substituents bonded to Se or S atom sterically reduce the possibilities of Se and S atoms to interact with species from the environment. The numerosity of crystal structures explains the lower values of O−H···Se (around −4.4 kcal/mol) and N−H···Se interactions (around −2.2 kcal/mol).

Acknowledgement: This study has been financially supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia.