Final project report KH 129588
"Supramolecular interactions in the solid state"

The aim of the project was the deeper understanding of supramolecular interactions to reveal their roles in the self-assembly of molecules in the solid phase. The investigation of non-covalent interactions is crucial in the understanding of the relationship between molecular structure and macroscopical properties, which is the key to the understanding of biological processes and of any types of application of materials like catalysts, chiral separation, molecular sensors, etc.

Since the supramolecular interactions are various, weak and numerous with limited directionality our goal was to investigate a wide variety of one and more component solid materials from biologically relevant organic molecules to metal coordination complexes in order to reveal their intermolecular features, to get inside into the packing arrangements of the molecules, to uncover why the specific crystal form or polymorphic forms appear. Our focus is not on the specific compound itself but on the intermolecular interactions it is able to form. We have synthetized a few of our investigated compounds (benzimidazole family, framework forming family), but many of them were made available in collaboration with national and international researchers for detailed structural investigations. We are grateful for our cooperating partners that they made us possible to perform detailed structural investigations of supramolecular aspects beyond a routine atomic structure determination. Structures, if they were available, from the Cambridge Structural Databank were also involved in the studies for comparison.

1. A significant research achievement was accomplished on the field of supramolecular interactions in the solid phase analysing crystal structures of 2-phenylbenzimidazole derivatives, either prepared by covalent synthesis by us or collected from the CSD. The molecular conformation of the flexible molecules and the placement of the molecules in the crystal lattice adjust to the supramolecular features. The deliberate fine tuning of structural properties was achieved by application of halogen substituents, changing its placement and/or chemical composition influencing electrostatic and sterical properties. We have revealed the limits of isostructurality by supramolecular interactions. The work was published [1] by invitation in themed issue of CrystEngComm "The Cambridge Structural Database - A wealth of knowledge gained from a million structures" celebrating the over one million crystal structures in the World. The article became a highlight paper and we have received the inside back cover page of this special issue. Avirmed Saranchimeg, Budapest University of Technology and Economics, graduated with her BSc thesis working on this topic. Two lectures were delivered at international conferences (South Africa, England on-line), two at Hungarian conferences (Debreceni Kerekasztal, HCS), and two posters were presented (New Zealand, San-Diego on-line). The project proved to be worth to continue in the future.

2. The intermolecular interactions were in the focus of our research, which determine the packing arrangement and influence the molecular conformation of flexible molecules. Investigation of supramolecular interactions may give explanation why the very same compound is able to arrange different ways in the solid phase, is able to build varying systems of supramolecular interactions, to understand the occurrence of polymorphs often with small free energy differences. We had three target compound families. The small molecule bis[diamminesilver(I)] sulfate [2] has a high (HT, above 83^{o}C) and a low temperature (LT) polymorphic modification. The structure of the HT form has not been known before. The standard heat of the formation of the LT form and the enthalpy of the polymorphic transformation were determined. The atoms became disordered, and the crystal symmetry becomes higher at higher temperature, while the change of the hydrogen bonds significantly alters the geometry of the complex cation. In case of four different benzyl-morpholino hydroquinone derivatives [3], developed for flow battery application, the aim of the structural investigation was to avoid the formation of the low solubility polymorph via understanding structure-property relationship. The structure of

Clopamide has not been published earlier, although it is a commercially available marketed diuretic. A method of single crystal growth was evaluated, and the structure of the anhydrate and hemihydrate crystal forms were determined [4]. It made possible to interpret the supramolecular role of the incorporating water molecule in the crystal lattice. Two newly defined secondary bond types: an intramolecular halogen bond and an intermolecular chalcogen bond were recognized in the structures. Forming the Cu(II) complex of Clopamide, four isostructural crystals using a homologous series of alcohols, three solvent-free polymorphic forms and one dichloromethane-containing solvatomorphic form were characterized to reveal the conformational differences of the molecule as an effect of the altering intermolecular interaction system in the crystals. These results bring us closer to the understanding of the supramolecular interactions which determine molecular recognition processes. Three invited lectures, two lectures at international conferences (Slovenia and Budapest) and one at a national event (HCS) were delivered on the aspects of supramolecular chemistry and polymorphism.

3. Electronic and steric structural directing effects were described used in inorganic crystal engineering in zinc(II) complexes with β-hydroxypyridinecarboxylate ligands keeping the supramolecular alternating arrangements in spite of the different coordination modes and complex geometries [5]. Based on this complex compound family, beside the published paper four talks were given at national conferences (Debrecen, HCS and HAS working committees), while it was also delineated in a poster (Vienna). Numerous metal complexes of 2-picolinic acid have significant pharmacological effect (low-to-moderate cytotoxic activity, insulin-mimetic activity, having low IC_{50} value, used as nutritional supplement for overweight people). We have examined the structural effect of the additional carboxyl group in the half-sandwich organometallic Ru(η^6 and η^5) 2,4-dipicolinate complexes and the lower affinity of the 2,4-dipic complexes to halide ions was found compared to the corresponding picoline complexes [6]. The effect of ligand methylation on solution speciation and anticancer activity of half-sandwich organometallic Ru and Rh complexes was investigated [7]. The studied complexes are highly stable, thus the liberation of the bidentate ligands is not likely. The change from p-cymene to toluene has only a negligible effect on the complex structure. The methyl groups distorted the structure, when they are present next to the coordinating atoms.

4. The number of crystal structures of diastereomeric salt pairs and especially of double salts is limited in the literature. We have exceptionally presented [8] the structures of two constitutional isomer double salts along with their related diastereomeric salt pairs (1-cyclohexylethylammonium 2-chloromandelate (S–S, R–S, SS–SR) and 1-cyclohexylethylammonium 4-chloromandelate (R–R, S–R, SS–SR)), which were successfully crystallized and their structures elucidated presenting two complete sets of chiral systems. These results provide a deeper insight into chiral recognition based on supramolecular recognition and contribute to the mastery of synthon engineering. One lecture at an international conference (Austria), one lecture at a Hungarian conference (HCS) and one poster presentation (Czech Republic) were delivered on this topic.

5. As it can be seen from the above list of compound families involved in our studies of supramolecular interactions in the solid state, a few compound families were accommodated to the project in addition to the original plans. Notwithstanding, we are behind of our planned schedule with two topics, both required extensive lab labour of syntheses and crystallization. Experimental work in the laboratories suffered more difficulties during the pandemic than the calculations. Anyhow, we are ready with the research work in both cases, we need to prepare the manuscripts. The results will be published in the near future. The NKFIH OTKA grant will be acknowledged in the papers.

Hydrogen bond assisted organic frameworks (HOF) proved to be ideal to study supramolecular interactions, symmetries and polymorphism. Synthesis of derivatives of the diazadibenzo[ef,kl]heptalene skeleton were performed in order to change the ring closure and ring substituents to influence intramolecular interactions which determine molecular rigidity; the substitution of the terminal phenyl rings to influence the spacer size and its intermolecular interactions, this way the

packing arrangement; and the incorporated charged sites to assist the strength of framework forming hydrogen bond as well. We are working on the manuscript revealing the conditions of the formation of the porous HOFs [9]. Preparation an investigation of HOF compounds is a brand new branch of chemistry, they are in the forefront of research interest. These materials still provide many challenges for the future, and it proved to be worth to continue the research on these compounds in the future. Lectures on the results were delivered at conferences in the UK, USA and Czech Republic.

The polymorphs and cocrystals of nitrofurazone (5-nitro-2-furaldehydesemicarbazone) a broad-spectrum bactericide is investigated to evoke different supramolecular interactions in order to lead to new solid forms with improved pharmacokinetic profiles. This project is being performed in international cooperation with Prof Nikoletta Báthori, CPUT, South Africa. The laboratory work was in delay because of the lock down in Cape Town. Anyhow, the research on nitrofurazone is completed, we need to write up the results [10].

The participants of the project remained the same during the three years as those in the funding contract. The focus of the project – supramolecular interactions in the solid phase - remained also the same throughout the years. The weight of importance of certain investigated compound families were shifted with the progress of the project based on the scientific outcome and the laboratory labour demand in the pandemic circumstances. In addition, new compound families were involved into the project.

Students:

In the first year of the project an MSc and three BSc students contributed mainly to the laboratory work, giving us the opportunity to make them familiar with the techniques of the single crystal growth, and to introduce them into the single crystal data collection.

One BSc student, Avirmed Saranchimeg, working on crystallization and structure solution and refinement of the benzimidazole compound family graduated from the Budapest University of Technology and Economics. The PhD thesis of Gyula Tamás Gál has been submitted to the György Hevesy Doctoral School of Chemistry, Faculty of Science, Eötvös Loránd University based on the complex compound families of this project. The poster he presented at the 32nd European Crystallographic Meeting was awarded the International Union of Crystallography Journal Prize for Strcutural Chemistry.

After the first year of the project recruiting and involvement of new students were hindered by the pandemic.

Publications:

The results are published in eight papers in international journals. It exceeds the formerly expected four to six papers. The sum of the impact factor of the journals is 26.0.

Two of the publications are invited papers. Ref 1 is an invited article to the themed issue on the occasion of the celebration of the one million structures in the Cambridge Structural Database with the title “The Cambridge Structural Database - A wealth of knowledge gained from a million structures”. Our paper became a highlight paper, and we were offered the inside back cover page. Ref 4 is an invited article to the themed issue “Host–Guest chemistry: in honour of Luigi Nassimbeni’s 9th decade, 2021” The paper is available on-line, the page numbers are expected in the coming days.

In addition to the eight published articles two more manuscripts are in due course of preparation where this grant will be acknowledged. Both topics demanded extensive synthetic labour in the laboratory where the pandemic introduced delay.

Conferences:

The pandemic prevented in person participation on scientific events from spring 2020. Since the restart of the conferences in the virtual world, the results were presented at on-line conferences. Before the pandemic an international and a national conference participation and a university visit were accounted to the project. Three participants of this project attended the annual crystallography meeting took place in August 2019 in Vienna. The second travel included almost all participants of the project: we have visited University of Vienna in November 2019 to get advice to our investment and to see how Raman microscope works in reality with crystallographic samples. This project financed the attendance of two participants at the on-line conference 4th International Symposium on Halogen Bonding in Stellenbosch, South Africa.

In total the results of the project were presented orally at eight international conferences (one of them was an invited plenary talk, one was an invited talk), and at nine national conferences (one was an invited talk). Six posters were also presented based on the results of the project at international conferences. One poster was awarded the Journal Prize of the International Union of Crystallography for Structural Chemistry.

Finances:

This project made possible two major investments in our laboratory.

A LINK-DV_HRC Image Capture Module and High Performance Digital Colour Camera was the investment of the project for brut 3.174.242 HUF in the first year. The camera is highly necessary to our work to project the view of the microscope to the screen and to follow the processes of crystal selection and record the stability investigations. This is a complex system, its software harmonises the shooting of the camera and the control of the hot stage also. Unfortunately, the controller of our hot stage went wrong completely beginning of the first year of the project and could not be repaired because the technology development (it is no more manufactured). There was no other way to make the hot stage operable than to purchase a new camera and computer software which controls and records what happens under the microscope. Although an X-ray sealed tube was planned originally as investment in the project. It is a regular need operating an X-ray apparatus. The investment of the project needed to be reconsidered because of the emergency situation to be able to continue our work. Since SXRD experiments are mostly performed at low temperature (-180^{o}C) to reduce thermal motions of the atoms and to reduce the presence of possibly occurring dynamically disordered atoms, therefore we need to check the crystals whether phase transition occurs during cooling, and to check crystal stability, decomposition, guest loss, melting in the -180 - +400 ^{o}C temperature range. The new system has been installed in our laboratory in the first year, payment was completed in the second year.

All the sources which were not or could not be spent mostly because of the pandemic were saved (rest of investment, consumables and conference participation) and it made possible to purchase an OptiprexxPLS Raman photoluminescence system for 7 045 771 HUF gross. The Raman spectrophotometer is suitable for polymorph investigations which depends on the different supramolecular interactions. Because of the very long ordering process (lockdown), although the equipment arrived in the second year of the project, the payment was arranged in the year of extension.

According to our plans we bought two computers for structural calculations with peripheries, and a NAS for data storage. Sets of erasing lamps to the diffractometer, maintenance of the chillers and UPS, ampoules, gas, compounds, solvents and stationeries were paid from the project.

The inside back cover page offered to our highlight paper was accounted to the project.

One participating researcher, Nagyné Bereczki Laura received salary supplement from this OTKA project.

This project provided the financial support to participate at an annual crystallographic meeting (ECM32 Vienna), and at a national conference (meeting of the HAS Working Committee on Material and Molecular Structure), as well as a visit to the Vienna University as a preparation of our investment before the pandemic. The participation on an international on-line conference (4-ISXB) was also covered by this project.

COVID

The Principal Investigator and the participating researchers are grateful to the NKFH for the grant what has made possible to perform the research summarized above. We are also grateful for the extension of the two year timeline with an extra year. The reorganisation of our research institution influenced our financial capabilities at the start of the project, then the lockdowns affected the progress of the research project both in performing the laboratory work and the investments. The pandemic had several different effects on the research:

- Recruiting and involvement of students to the work become embarrassed
- Lab availability was restricted for us because of the limited number of people could stay in the same lab at the same time. Lab access was prohibited in some countries including our collaborating partner
- The pandemic slowed down the investment, and acquisition in general.

As this grant was provided for a short two year period, the year of extension made possible to complete the publication process of eight papers (two more publication are expected) and a PhD thesis.

Exploitation:

The research of supramolecular interactions is basic research that is necessary to use in applied research and innovation. It reveals the relation between the molecular structure and the physical and chemical properties. Application of the principles of molecular recognition is crucial in the forecasting of biological activity and in any material science application. This knowledge is inevitable in pharmaceutical research, and in the development of new materials with desired new properties, like catalysts, fertilizers, pesticides, inks, paints, electronic, optical and energetic materials.

Budapest, 29th October 2021

Petra Bombicz

Principal Investigator

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Publications:

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    in preparation

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