APPENDIX No. 4

Summary of professional accomplishments with the list of published scientific papers or creative professional work, and information on teaching achievements, cooperation in science and popularization of science

I. Summary of professional accomplishments

1. Name.

Paulina Maria Dominiak

2. Held diplomas, scientific / arts degrees - with the name, place and year of acquisition, and the title of doctoral dissertation.

Doctor of chemical sciences in the field of chemistry, Department of Chemistry, University of Warsaw, Warsaw, 12.01.2005
"*Weak Interactions at Different Levels of Complexity in the Solid State*"
(pol.: „*Słabe oddziaływania na różnych poziomach organizacji materii w fazie stałej"*)

Master of Chemistry, Department of Chemistry, University of Warsaw, Warsaw, 4.07.2001

Master of Biology (with specialization in molecular biology), Department of Chemistry, University of Warsaw, Warsaw, 28.06.2000

3. Information on current and previous employment in scientific /art institutions.

since 02.2007	Department of Chemistry, University of Warsaw, Warsaw, Poland, Associate Professor (pol.: adiunkt)
01.2005-12.2006	Department of Chemistry, State University of New York at Buffalo, Buffalo, NY, USA, Postdoctoral Research Associate & Research Instructor (pol.: staż podoktorski)

4. Indication of achievement[1] under Art. Paragraph 16. 2 of the Act of 14 March 2003 Academic Degrees and Title, and Degrees and Title in Art. (Dz. U. No 65, item. 595 with amendments.):

a) the title of the scientific / artistic achievement,

"Databank of Aspherical Atoms and Its Role in Crystallography and Structural Biology"

[1] if this is the achievement of joint publication / publications, provide a declaration of all its coauthors, determining the individual contribution of each of them in its creation.

b) publications comprising the academic achievement

H1. Dominiak* P. M. & Coppens* P., **2006**, *Finding optimal radial-function parameters for S atoms in the Hansen–Coppens multipole model through refinement of theoretical densities*, **Acta Crystallogr**. *A62*, 224-227.

H2. Dominiak* P. M., Volkov* A., Li X., Messerschmidt M. & Coppens* P., **2007**, *Theoretical Databank of Transferable Aspherical Atoms and Its Application to Electrostatic Interaction Energy Calculations of Macromolecules*. **J. Chem. Theory Comput.**, *3*, 232-247.

H3. Dominiak* P. M., Volkov A., Dominiak A. P., Jarzembska K. N. & Coppens* P., **2009**, *Combining crystallographic information and an aspherical-atom data bank in the evaluation of the electrostatic interaction energy in an enzyme-substrate complex: influenza neuraminidase inhibition*. **Acta Crystallogr**. *D65*, 485-499.

H4. Bąk J. M., Dominiak P. M., Wilson C. C. & Woźniak* K., **2009**, *Experimental charge-density study of paracetamol – multipole refinement in the presence of a disordered methyl group*, **Acta Crystallogr**. *A65*, 490-500.

H5. Bąk J. M., Domagała S., Hübschle C., Jelsch C., Dittrich B. & Dominiak* P. M., **2011**, *Verification of structural and electrostatic properties obtained by the use of different pseudoatom databases*, **Acta Crystallogr**. *A67*, 141-153.

H6. Jarzembska* K. N. & Dominiak* P. M., **2012**, *New version of the theoretical databank of transferable aspherical pseudoatoms, UBDB2011-towards nucleic acid modelling*, **Acta Crystallogr**. *A68*, 139-147.

H7. Bąk J. M., Czyżnikowska Z. & Dominiak* P. M., **2012**, *Is it possible to derive quantitative information on polarization of electron density from the multipole model?*, **Acta Crystallogr**. *A68*, 705-714.

H8. Woińska M. & Dominiak* P. M., **2011**, *Transferability of Atomic Multipoles in Amino Acids and Peptides for Various Density Partitions*. **J. Phys. Chem. A**, *117*, 1535-1547.

c) discussion of the scientific / artistic goals of the above publication / publications and the results achieved together with a discussion of their possible use.

1. Scientific Goal

The main idea of the above-mentioned series of publications was **the development and validation of new scientific method** to be used in X-ray crystallography. The method is based on a bank of fragments of atomic electron densities. Some applications of the newly created method go, however, far beyond crystallography.

The electron density is a key factor in determining properties of molecules. Knowledge of the electron density distribution allows us to determine the three-dimensional structure of molecules (chemical bond lengths, valence angles, the absolute configuration, etc.), and various one-electron properties (electric moments, electrostatic potential, electrostatic interaction energy, etc). X-ray diffraction with molecular crystals is a great tool for obtaining this kind of information. In addition, information about intermolecular interactions becomes available.

X-rays are diffracted by the electron density of crystals. Thus, the correct analysis of the single crystal X-ray diffraction pattern can provide information about the distribution of charge density. How precisely and accurately we are able to determine the electron density distribution of a crystal is largely determined by **the resolution** of the diffraction data collected. In the case of crystals of small molecules, the majority of X-ray diffraction data are collected at the standard resolution d_{min} = 0.84 Å. Crystals of proteins and other macromolecules diffract most frequently to d_{min} = 2.1 Å, although the number of atomic resolution data (*i.e.*; greater than approximately 1.0 Å) is constantly growing. Only in the case of one crystal per thousand, predominantly of crystals of small molecules, is the quality good enough to enable analysis of the diffraction data at the subatomic resolution, *i.e.*; about 0.45 Å. Subatomic resolution is necessary to determine the distribution of electron density in a quantitative manner.

In analysing the diffraction data it is necessary to use a predetermined **model of the electron density distribution** to be able to get rid of the artefacts resulting from experimental errors, lack of the structure factor phases, and a finite number of measured reflections. Only selected parameters of a given model are refined against the experimental data. In a typical X-ray analysis, small molecules (and protein) crystallography, the electron density of the crystal is modeled by the sum of the contributions of the individual atoms. Individual atoms are represented by the spherically averaged electron density distributions obtained by theoretical methods for isolated atoms in the ground state. This is called **the independent atom model** (**IAM**). The assumption that the electron density of the crystal is dominated by the density centered around the cores of atoms and that the electron density maxima coincide with the positions of atomic nuclei is used here. Using this model, the average positions of atoms in the unit cell (x, y, z) and the parameters describing the displacement of the atoms from their average position (so-called atomic displacement parameters, ADPs) are refined against the experimental data (more precisely, the measured intensities of reflections). In the case of proteins and other macromolecules, the typical data resolution is so small that additional constraints are used in the refinement of the above-mentioned parameters in order to compensate for the lack of sufficient data. The IAM model does not take into account changes in the density distribution of individual atoms due to phenomena such as formation of chemical bonds, charge transfer, lone electron pairs, etc. The information obtained in this type of analysis is therefore only **the geometrical information** of the crystal structure. At the same time, the geometrical parameters so derived are subject to some systematic errors.

The most well-known artefact of the standard X-ray data is the significantly underestimated length of the X–H bonds (X – non-H atom). Hydrogen atoms do not have core electrons and the valence density is strongly shifted towards the center of the bond. Another possible systematic error is overestimation of the values of atomic displacements parameters, ADPs. Deficiencies in the IAM model can also appear on the Fourier difference maps (maps obtained by Fourier synthesis of the differences between the experimental structure factors and the structure factors calculated on the basis of the refined model). Lone electron pairs and bonding electron pairs not described by the model remain in the difference map, Fig. 1.1. Therefore, for a measurement of sufficient quality, in which the intensity of reflection errors are correctly estimated, the goodness of fit of the model (GooF) for the unweighted reflections is still far from the desired value of unity.

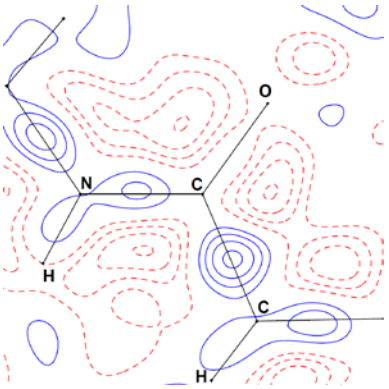

Fig. 1.1. An example of the Fourier difference map F_o–F_c for X-ray diffraction data of resolution d_{min} = 0.84 Å refined with the IAM model (F_o – experimentally observed structure factors, F_c – structure factor computed from the model). Contours: every 0.025 e/Å^3, positive – blue, negative – red.

Progress in measurements and computational techniques of X-ray diffraction made most routine diffraction measurements on single crystals of small molecules (i.e. measurements of the resolution $d_{min} \leq 0.83$ Å as recommended by the International Union of Crystallography) good enough to see all of the above systematic errors caused by the IAM model. Therefore, there is a need for a new, more realistic model of the electron density. It would have to be a model taking into account the asphericity of atoms in a molecule/crystal and having parameters that describe the change in the density distribution of the atom due to the formation of bonds and other interactions with neighboring atoms.

Unfortunately, only at subatomic resolution does the number of the collected data allow refinement of more parameters than is in the case for the IAM model. With high-resolution data, instead of the spherical IAM model, **a multipole model** of the atom electron density is most often used. In the multipole model, atoms are represented with a finite spherical harmonic expansion of the electron density around each atomic center. This expansion is called a pseudoatom. In a commonly-used variant of the multipole model, the so-called Hansen-Coppens model [1], the electron density of a pseudoatom is defined by:

$$\rho_i(\boldsymbol{r}) = \rho_{core}(r) + P_v\kappa^3\rho_{valence}(\kappa r) + \sum_{l=1}^{l_{max}} \kappa'^3 R_l(\kappa'\zeta r) \sum_{m=0}^{m=l} \sum_{p} P_{lmp} d_{lmp}(\theta,\phi)$$

$$R_l(\kappa'\zeta r) = (\kappa'\zeta)^3 \frac{(\kappa'\zeta r)^{n_l}}{[n_l+2]!} exp(-\kappa'\zeta r)$$

where $\rho_{core}(r)$ and $\rho_{valence}(r)$ are spherically-averaged free-atom core and valence densities normalized to one electron, respectively; $R_l(\kappa'\zeta r)$ is a Slater type radial function with predefined values of ζ and n_l parameters; and $d_{lmp}(\theta,\phi)$ (p= ±) are density-normalized real spherical harmonic functions. The coordinates r, θ, ϕ refer to a local cartesian coordinate system centered on the atomic nucleus. The populations P_v and P_{lmp}, and the dimensionless expansion-contraction parameters κ and κ' are refined against experimental data, in

addition to the above-mentioned parameters describing the positions of atoms (x, y, z coordinates and ADP parameters). Such a model, after refinement, provides **quantitative information about the electron density** distribution of the crystal. Consequently, more precise positional parameters of atoms are obtained which leads to more precise bond lengths, for example. It becomes possible to perform topological analysis of the electron density distribution (and other functions derived from it) in the light of the theory of Bader's QTAIM (Quantum Theory of Atoms In Molecules) [2]. One can attempt to calculate atomic and molecular properties such as: charge; dipole and higher electric moments; the electrostatic potential of molecules; and the energy of electrostatic interactions between molecules. At the same time, using this model one should also be aware of its limitations [3, 4], some of which will be discussed later in this text.

At this point, it is worth mentioning some later-introduced alternatives to multipole refinement, such as: the X-ray constrained Hartree-Fock (XCHF) modeling [5], molecular orbital occupation number (MOON) refinement [6] and the maximum entropy method (MEM) [7].

Ideally, all the X-ray structural measurements would be high-resolution. In practice it is not easy to achieve subatomic resolution. Not all crystals are of sufficient quality, and not all scatter X-rays with sufficient intensity at high diffraction angles. Not all single crystal X-ray diffractometers are sufficiently accurate. The fact that high-resolution measurements are labor- and time-consuming, or simply much more expensive than the standard measurements, cannot be ignored either.

It has been noted that the values of pseudoatom parameters are almost identical for atoms in similar chemical environments [8], i.e. atoms having similar local topology of connecting chemical bonds. One idea is to build a databank of different types of pseudoatoms and to use the bank to create a **transferable aspherical atom model (TAAM)** for any organic molecules, including proteins and nucleic acids. Replacement of the IAM model by TAAM in the refinement procedure of standard diffraction data should lead to more accurate geometrical information and provide access to quantitative estimation of the electron density distribution and properties derived from it (dipole moment, electrostatic potential, etc.) for molecules in a crystalline environment.

Pioneering work towards building a pseudoatom databank from experimentally determined electron densities have been published in 1995 by the group of prof. Lecomte' [9]. In 2002, Koritsanszky, Volkov and Coppens [10] proposed the construction of an aspherical pseudoatom databank based on theoretically-calculated structure factors. Two years later, the first official version of the theoretical pseudoatom databank constructed in the group of prof. Coppens was released [11]. At the same time, Dittrich from the group of prof. Luger proposed an alternative theoretical databank of pseudoatoms [12]. To this day, all three databanks are being developed:

- ELMAM (Experimental Library of Multipole Atoms Model) [9, 13, 14];
- Invariom (INVARIant atOM) databank [12, 15]; and
- UBDB (University at Buffalo DataBank) [10, 11, H2, H6].

At the same time, there has been discussion in the literature on the advantages and disadvantages of using the above databanks [16].

In 2005, during my post-doctoral work in the laboratory of Prof. Coppens, I took over the development of the UBDB. Since my return to Poland (2007), the UBDB has been solely developed in my research group, i.e. with the help of graduate students under my direct supervision within the research team headed by Prof. Krzysztof Woźniak.

My specific scientific objectives were:

- Expansion of the UBDB for all atom types present in natural amino acids, proteins, nucleic acids and other biologically important molecules [H2, H6]. Optimization of the algorithm that defines the atom types and optimization of the method used to reconstruct the electron density [H1, H2, H6, H7, H8].
- Verification of the quality of electron densities reproduced by the UBDB by comparing them with quantum chemical results using the example of a large set of model polypeptides and short fragments of nucleic acids. In particular, verification of the quality of the intermolecular electrostatic interaction energies [H5, H6].
- Verification of the applicability of the UBDB as a source of aspherical scattering factors for the analysis of X-ray diffraction data at various resolutions [H4, H5].
- Comparison of the results of the UBDB applications with the results obtained using other databanks developed worldwide (ELMAM and Invariom) [H5].
- Testing of the usefulness of the UBDB in studying biological molecules of importance in medicine or biotechnology [H2, H3].

2. Results

a. The University at Buffalo Data Bank (UBDB) of aspherical pseudoatoms

In 2005, the UBDB contained about 37 atom types based on about 46 molecules. Preparing the next versions of the databank required verification and automation of procedures leading to the creation of new atom types; redefinition of keys based on which atom types are recognized; redefining how local coordinate systems for particular atom types are to assigned; redefinition of the averaged neutron X-H bond lengths according to the recently-published work of Allen and Bruno [17]; and modification of the LSDB program code (originally written by Dr. Volkov). Two further versions of the databank have been published: in 2007 [H2] and in 2012 (with the participation of my PhD student Katarzyna Jarzembska; [H6]). Currently, the UBDB includes more than 200 atom types of elements such as C, H, N, O, S, P, B, F, Cl and I, and is based on the electron densities of more than 600 molecules. The databank contains all the atom types necessary to describe proteins and nucleic acids, as well as many other biologically important molecules. The latest version of the UBDB and the LSDB program necessary for the databank application is available on the website http://crystal.chem.uw.edu.pl.

In the UBDB, each atom type results from averaging of density parameters (P_v, P_{lmp}, κ i κ') for the entire family of pseudoatoms being chemically equivalent. Density parameters are obtained by fitting in Fourier space the multipole model to the molecular density determined by the quantum-mechanical methods for a series of small molecules. In the definition of different atom types both the first and the second neighbors are involved, and statistical methods are used to allow the control of the density parameters' transferability. Details of the procedure for constructing the databank are given in H2 and H6, and schematically shown in Fig. 2.1. A set of keys necessary to define the atom type is shown in Fig. 2.2. Examples of deformation densities (electron density of pseudoatomu/ molecule minus spherically averaged electron density of the isolated atom/ -s) for selected atom types and a subsequently-reconstructed molecular deformation density are shown in Fig. 2.3.

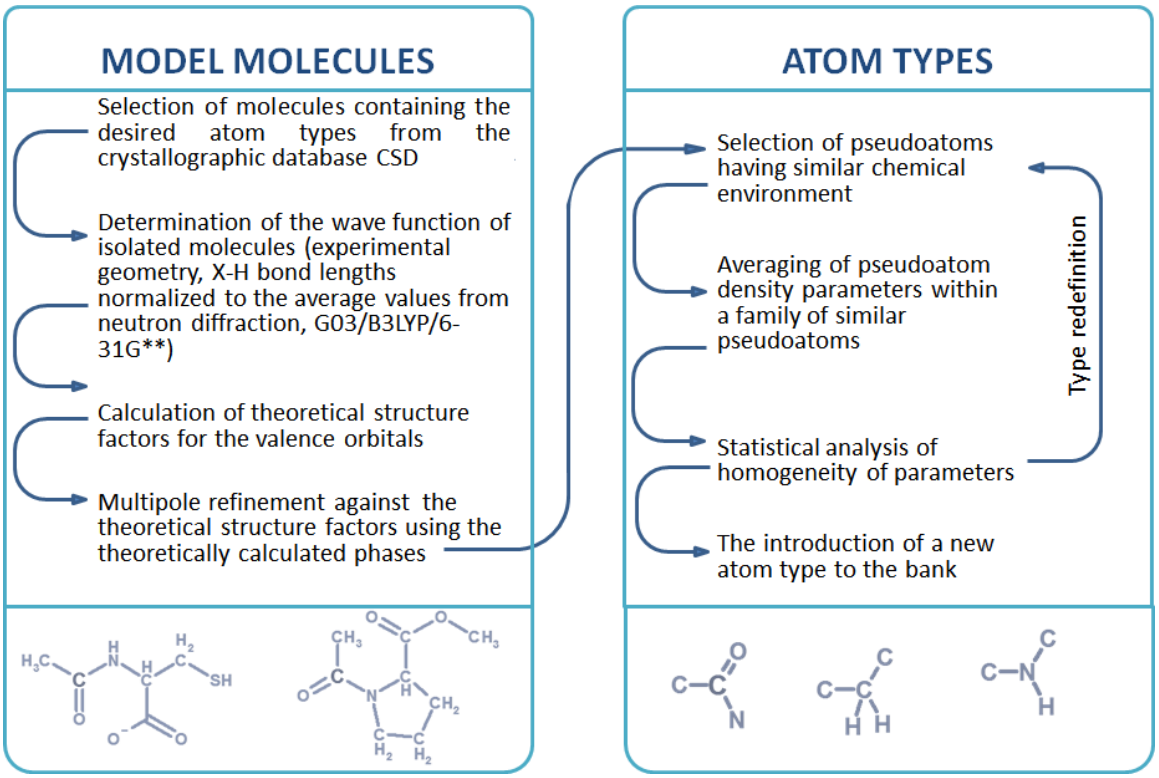

Fig. 2.1. Schematic procedure for building the UBDB.

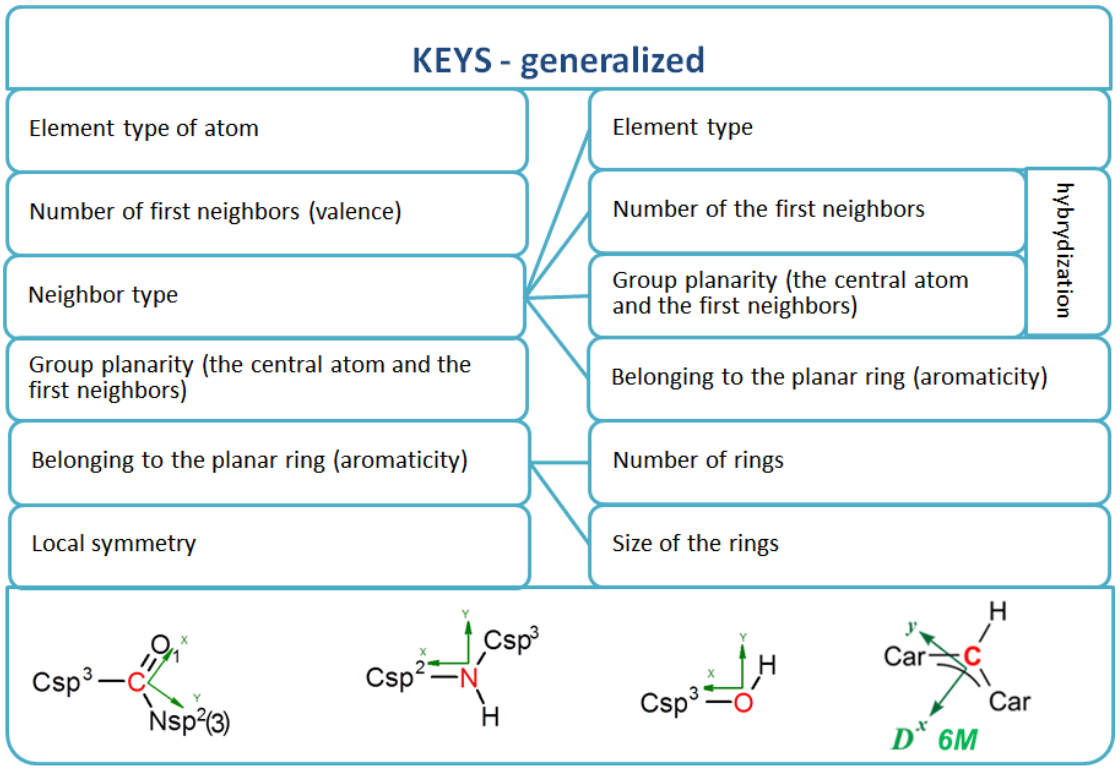

Fig. 2.2. Scheme of keys necessary to define atom types - generalized.

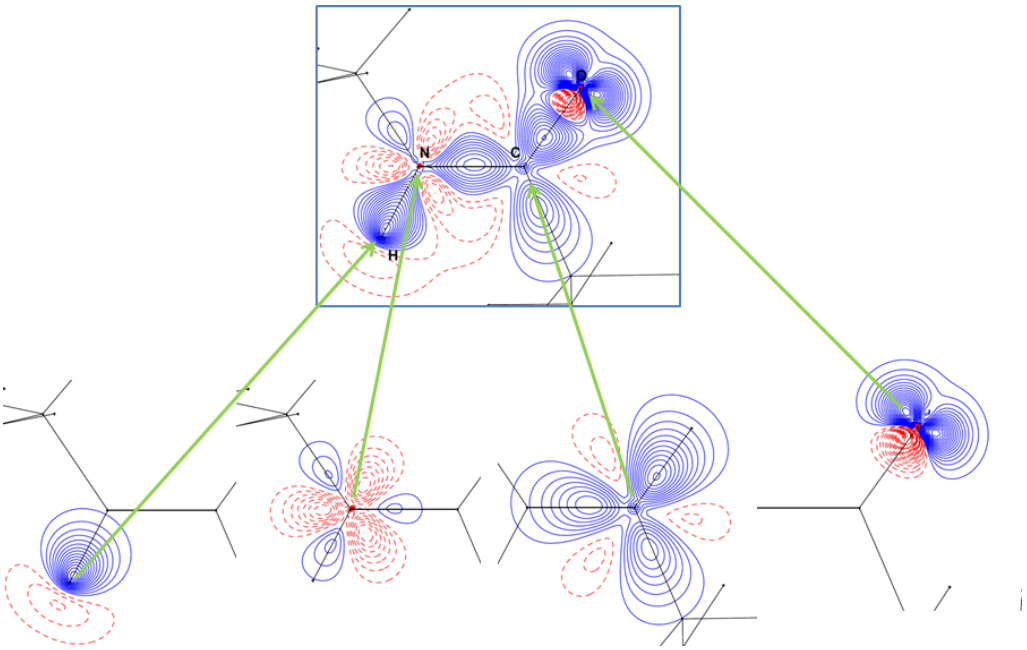

Fig. 2.3. Deformation densities of the sample atom types and deformation density of the reconstructed fragment of the molecule (peptide bond). Contouring in increments of 0.05 e/Å^3, positive – blue, negative – red.

Expanding the databank with new atom types of elements such as sulfur and phosphorus required modification of parameters in the standard multipole model. Optimization of n_l parameters of the radial functions from deformation part, $R_l(\kappa'\zeta r)$, significantly improved the fit of the multipolar model to the theoretical molecular densities. In the case of sulfur atoms, optimal values were shown to be 2, 4, 6, 8, respectively for n_1, n_2, n_3, n_4. For the phosphorus atoms optimized values are $n_{1,\ldots,4}$ = 6, 6, 6, 6. Details of the optimization procedure are given in H1.

The key concept for building any kind of databank of atom types is **transferability**. The level of transferability of the pseudoatomic electron density (and derived properties such as charge, for example) is affected by:

- conformational invariance *i.e.*, sensitivity of the electron density of a given atom type to conformational change of the molecule (transferability within the same molecule);
- invariance of the electron density of atoms having similar topology of chemical bonds (chemical environment), *i.e.*, the sensitivity of the electron density to changes in the nearest chemical environment (transferability between molecules);
- intermolecular interactions (transferability between complexes of molecules/ crystals);
- the method of defining an atom type, *i.e.*, the type of parameters/ keys used to uniquely define the type — the definition of the nearest chemical environment;
- the method of partitioning the molecular/ crystal densities into atomic contributions.

All these phenomena have been studied in the context of the UBDB creation.

Conformational invariance of pseudoatoms having the same chemical surroundings has been studied by Koritsanszky and co-authors [18]. Based on the electron density of the Ala-Ser-Ala tripeptide, Koritsanszky concluded that the variability of pseudoatom density parameters describing backbone atoms of the central amino acid residue is relatively small (which is usually up to 10% with respect to the mean values), and that is comparable to the variation generated by changes in the amino acid sequence.

Influence of the chemical environment on pseudoatom parameters transferability is constantly monitored during the construction of new atom types in the UBDB. This is possible thanks to the fact that the density parameters for each atom type are obtained by averaging the set of density parameters of individual pseudoatom coming from different model molecules. In accordance with the spawning procedure which I proposed [H2], values of pseudoatom parameters within the family of pseudoatoms having similar chemical environments are analyzed in terms of homogeneity of the sample. It is checked whether the distribution of these values is unimodal, or, on the contrary, whether there are two or more clusters of values. If it is possible to define the chemical reason (such as the different nature of the third neighbor), for which the value of any of the parameters differentiate, a set of keys used in the definition of the atom type is redefined (eg., new keys are added). In this way, on the basis of the given family of pseudoatoms, instead of one, two or more atom types are formed. There is also possibility to combine the two atom types, for which there are no statistically significant differences in the average values of any density parameters. Through this procedure it was found, for example, that the nitrogen atoms in their role as first neighbors need to be further characterized by providing information whether they belong to the planar group or not [H2]. Also, it became clear that atoms belonging to the planar rings should be additionally characterized by information about the size of the ring [H6].

Intermolecular interactions may significantly affect the distribution of the electron density of atoms directly involved in them. However, the matter of quantitative description of these changes in density described by the Hansen-Coppens multipole model was subjected to discussion in the literature [4]. Therefore, before attempting to quantitatively characterize the influence of intermolecular interactions on the transferability of pseudoatom density parameters, together with a doctoral student working under my direct supervision Joanna Bak, we decided to independently verify whether the multipole model is able to quantitatively describe intermolecular interactions [H7]. As a reference point, we chose theoretical electron density distributions of amino acids (D, L-His and L-Ala) and dipeptides (Gly-L-His, L-His-L-Ala) computed for isolated molecules and molecules surrounded by point charges, dipoles and quadrupoles located at positions of atoms of neighboring molecules (simulation of interactions in the crystal, the details of procedures are given in H7). Our research has shown that the Hansen-Coppens multipole model only reflects in a qualitative way the changes in molecular electron density due to polarization by the neighboring molecules, and just in the area of bonds and lone electron pairs. The multipole model is unable to describe the changes in the vicinity of the atomic nuclei. In the case of properties derived from the multipole model, such as dipole moment and electrostatic energy of interaction between molecules, changes due to polarization are not reproduced, even in a qualitative manner. Any attempt to build a databank that describes polarization present in the intermolecular interactions must therefore wait until a better pseudoatom model is introduced.

In search of a way to improve the transferability of pseudoatom parameters, I asked myself whether it is possible to further increase the transferability by changing **the method of partition of molecular/ crystal density** into atomic contributions. After a series of calculations for a set of ten selected amino acids and some di-and tripeptides composed of them, together with my postgraduate student Magdalena Woińska, we concluded [H8] that the Hirshfeld partition [19] yields slightly better transferability of the electric moments of atoms when compared to partition by fitting the Hansen-Coppens multipolar model to the density or the atomic basin partition in the light of the QTAIM theory. This opens the way to design better procedures for creating pseudoatom databanks. Many other researchers also

prefer Hirshfeld partitioning [20].

b. Verification of the quality of electron densities reproduced by the UBDB

Molecular electron densities reconstructed using the first version of the UBDB [11] were initially verified by Volkov et al using six test small molecule crystal structures (mainly amino acids) [11, 21] and seven fragments of vancomycin complexes with small ligands [22]. The authors compared the deformation density maps, molecular electrostatic potential mapped on the electron density isosurfaces (MEPS), local and integrated topological properties of the electron density and the electrostatic energy of intermolecular interaction (E_{es}), using the results of high-quality quantum chemical calculations as a benchmark. They concluded that the databank satisfactorily reproduced all the properties tested.

To verify the new versions of the UBDB, we decided to focus mainly on the **electrostatic energy**, E_{es}, as it is the one-electron property which was found to be most sensitive to any imperfections in the reproduction of the charge density distribution. In addition, the ability to accurately assess the electrostatic contribution to the energy of interactions seems to me a very attractive and important feature of the UBDB, allowing applications far beyond crystallography. Reconstructing the electron density of the molecules with the UBDB and using the EPMM method (Exact Potential/ Multipole Method) [23] to calculate the energy, one can quickly obtain the E_{es} energy directly corresponding to $E_{pol}^{(1)}$ in the Symmetry-Adapted Perturbation Theory (SAPT) [24]. E_{es} is therefore the classical coulombic electrostatic interaction energy of the unperturbed charge distributions of molecules A and B forming a complex A:B. It is worth noting that such a definition already takes penetration into account, which is neglected in a simplified method of E_{es} calculation based only on point electric moments as carried out by traditional force fields [P34]. For more than 190 complexes of nucleic acid basis, amino acids, peptides, and nucleic acid bases interacting with amino acid residues, together with doctoral students Katarzyna Jarzembska and Joanna Bąk, we showed that E_{es} values calculated using the method UBDB + EPMM strongly correlate with the reference values, the RMSD (Root-Mean-Square-Difference) for the total sample is approximately 3.6 kcal/mol with respect to E_{es} calculated using quantum chemical methods at the B3LYP/6-31G** level, Fig. 2.4. Details of the calculations and the detailed results, including the estimation of dipole moments and MEPS, and comparisons with higher-level quantum chemical calculations are given in H5 and H6. In addition, together with doctoral student Prashant Kumar working under my direct supervision and my graduate student Sławomir Bojarowski, we made comparisons of results from this method with the values of E_{es}, MEPS and the dipole moments of small of molecules (test sets: S66, S22 and JSCH-2005 from the laboratory of Prof. Hobza [25]) calculated using the selected force fields (Amber, CHARMM, OPLS) [26].

All the tests we have performed clearly show that, using the UBDB, one can:

- in a very fast way reconstruct the electron density distribution and perform calculations for large systems (eg., protein complexes), for which the use of quantum chemical methods is practically impossible;
- the results are qualitatively (and quantitatively) close to those of quantum chemical methods and at the same time are better than those of conventional force fields.

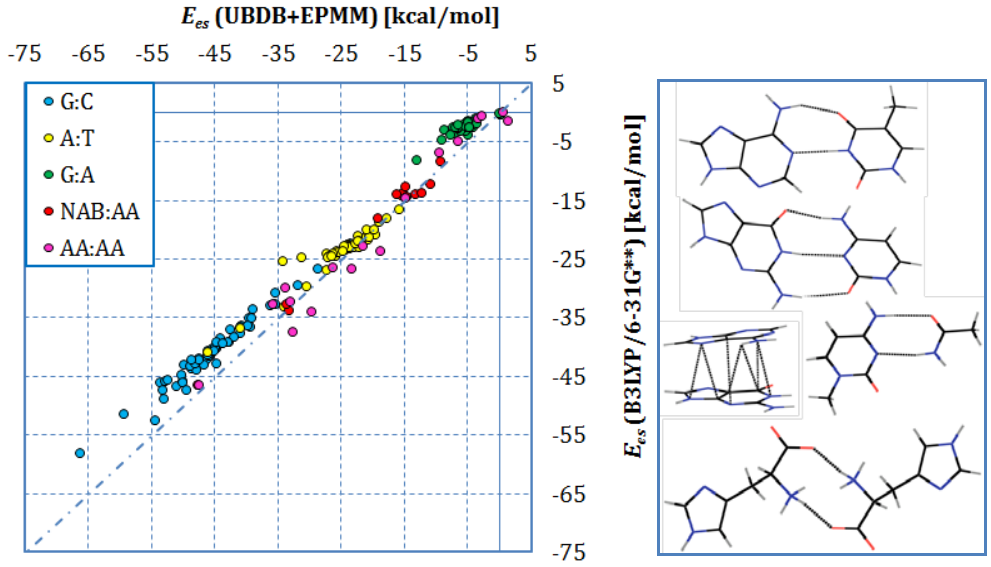

Fig. 2.4. *Left*: Values of E_{es} [kcal/mol] calculated using the method UBDB + EPMM with reference to the results from the quantum chemistry methods at B3LYP/6-31G** level. *Right:* Selected examples of complexes for which the E_{es} energy was calculated.

c. Verification of the applicability of the UBDB as a source aspherical scattering factors for X-ray data analysis.

The first tests of UBDB applicability in the refinement of **standard-resolution X-ray data** were carried out by Volkov et al [27] for Tyr-Gly-Gly ·H_2O and cyclo-(D,L-Pro)$_2$-(L-Ala)$_4$·H_2O crystals. They demonstrated that the use of a TAAM model built using the UBDB, when compared to the IAM model (a) significantly decreases the conventional *R*-factor, and density maxima at bond positions are no longer visible on the Fourier difference maps; (b) improves the geometry of molecules and the description of atomic displacements; (c) the values of the structure factor phases and the overall scale factor are closer to those corresponding to full multipolar refinement of high resolution data.

Our additional tests, carried out together with my PhD student Joanna Bąk, for two sets of X-ray data of standard resolution (d_{min} = 0.7 Å) collected for crystals of L-His-L-Ala ·2H_2O o and L-Ala confirmed that the TAAM refinement [H5]:

- improves the values of statistics describing the overal fit of the model to experimental data, for example, reduces the conventional *R*-factors (R_f, wR_f, R_{f2}, wR_{f2}) by about 1%; values of GooF become significantly closer to unity;
- reduces the values of the density maxima and minima, and randomizes their location on Fourier difference maps, Fig. 2.5;
- significantly improves the position of the hydrogen atoms (when freely refined). For example, the resulting X-H bonds are longer by about 0.1 Å, and differ only by an average of 0.02 Å from the reference structures (from neutron diffraction data or those obtained from the optimization of the geometry of the periodic system) , Fig. 2.6:
- significantly improves the parameters of anisotropic ADPs for non-hydrogen atoms. For example, there is an approximately 10% reduction in the values of the ADP parameters relative to the IAM refinement, and the obtained values of the parameters differ by about 3% compared to those from full multipole refinement against high-resolution data ($d \leq$ 0,45 Å).

Currently, in collaboration with prof. Coppens and prof. Adams (Lawrence Berkeley Laboratory, Berkeley, CA, USA), we are conducting tests on TAAM refinement of

macromolecular X-ray data (proteins and nucleic acids).

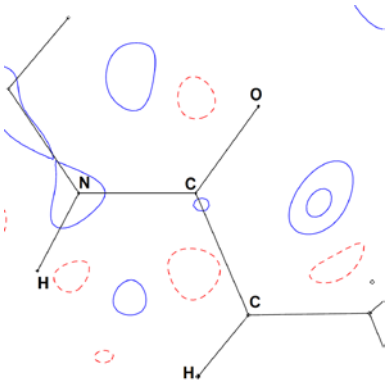

Fig. 2.5. An example of the Fourier difference map F_o–F_c for X-ray diffraction data of resolution d_{min} = 0.84 Å refined with the TAAM model (F_o – experimentally observed structure factors, F_c – structure factor computed from the model). Refinement was carried out with the same data as for the case presented in Fig. 1.1.Contours: every 0.025 e/Å^3, positive – blue, negative – red.

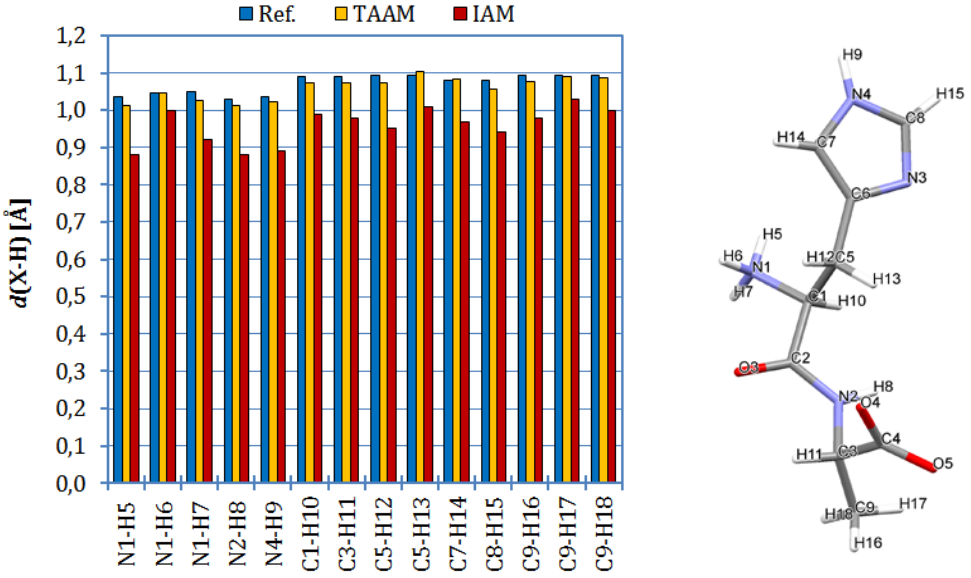

Figure 2.6. Sample X-H bond lengths [Å] (X is non-H atom) from X-ray data of resolution d_{min} = 0.84 Å refined with the IAM (red) or TAAM (yellow) model, compared to the reference lengths (blue) obtained from optimization of the geometry of the periodic system (CRYSTAL06/B3LYP/DZP).

The UBDB can also be used as **a starting multipole model** for full multipole refinement of X-ray data of the sub-atomic resolution. In multipole refinements, one of the key problems is the correct deconvolution of the thermal vibration of the atoms (modeled by ADP parameters) from the static electron density (modeled by multipole model parameters). Our tests show that the ADP parameters for non-hydrogen atoms obtained in the TAAM refinement of high-resolution data constitute a very good **starting model of atom displacements** in multipole refinement [H5].

We have also, together with doctoral student Joanna Bąk, tested the UBDB applicability to **high-resolution data refinement** [H4] of X-ray data collected for crystal of one of the paracetamol polymorphs which exhibit dynamic disorder of the methyl group. Until now it was believed that it is not possible to obtain the correct distribution of the electron density for disordered crystals. The use of the databank to model the density of the methyl group and the κ '- constrained multipolar model refinement of the remainder atoms

of the molecule allowed us to obtain a reliable model of the density distribution of the crystal.

d. Comparison of the results of UBDB applications with the results obtained by using Invariom and ELMAM databanks.

I believe that a great success was to bring about a precise comparison of all three competing pseudoatom databanks [H5]: ELMAM (and later ELMAM2), Invariom and UBDB. With the doctoral student Joanna Bąk we showed that there is **no practical difference** among the databanks in terms of their use **as a source of aspherical scattering factors** in TAAM refinement. All three databanks lead to a similar quality of structural data, and all have the same advantage over the IAM model.

Each of the tested databanks may, after the TAAM refinement of high-resolution data, lead to a very good starting multipole model of the static density and starting model of thermal vibrations.

Quantitative comparison of **the properties** that are derived **from the reconstructed densities**, such as the deformation density, dipole moments, statistical characterizations of MEPS and interaction energies E_{es} for dimers of molecules shows that the analyzed databanks are **significantly different** from each other. Comparison of the E_{es} values to the results of quantum chemistry calculations (at different levels) suggests that the **UBDB** is slightly better in this regard than other banks: RMSD values for test systems for the **UBDB** are in the range of 2-3.5 kcal/mol, and for the other banks in the range of 5-8 kcal/mol.

e. Usefulness of the UBDB in studying biological molecules

The potential of the UBDB as a tool for the analysis of protein interactions in their complexes is illustrated by the results of my work on the complexes of the second PDZ domain of syntenin [H2] and on *Influenza* neuraminidase complexes [H3].

PDZ domains are structural domains widely present in signaling proteins of most living organisms. In general, the PDZ domains bind short C-terminal fragments of the peptide chain of specific proteins. The binding occurs by building an extra β-strand on the existing PDZ domain β-sheet. The side chains of amino acid residues at P_0 and P_{-2} positions in the target protein (P_0 and P_{-n} denote the C-terminal amino acid residue of the bound protein and the *n*t-h upstream amino acid residue, respectively) are responsible for the specificity of the PDZ domain. Motifs recognized by the PDZ domain are divided into three main classes: type I of the consensus sequence −(S/T)XΦ; type II with –ΦXΦ and type III with −(D/E)XΦ, where X is any amino acid, Φ is an amino acid with hydrophobic side chain, S/T is either serine or threonine and D/E is glutamic or aspartic acid. There are, however, many exceptions to the proposed classification. The second PDZ domain of syntenin, for example, exhibits degeneration of specificity. It has been shown that it is able to bind peptides belonging to both types, type I and II. Analysis of electrostatic interactions in eight complexes of the syntenin PDZ2 domain (Fig. 2.7), which I carried out using our UBDB+EPMM method, explains the energetic basis of that domain degeneration of specificity. The E_{es} energy of interaction of PDZ domain with −DSVF tetrapeptide belonging to type I is very similar to the interaction energy for –EFYA, −EYYV and –EYKV peptides of type II, all of them equal on average to -110 kcal/mol. The other two peptides of type II, −EFYF and –EFAF, interact a little more strongly, E_{es} is about -135 kcal/mol. Analysis of the contribution of each position in the peptide revealed:

- phenylalanine at the P_0 position (regardless of type), interacts more strongly with the PDZ domain (by about 20 kcal/mol) than the other amino acids in this position,
- serine (type I) at the P_{-2} position interacts less strongly (by about 10 kcal/mol) than the

hydrophobic residues present at the same position in the type II peptides;

- amino acid residues at the P_{-1} position practically does not interact;
- a strong interaction of the side chains of aspartic or glutamic acid residues is observed at the P_{-3} position, a position which so far was not taken into account in the literature.

The first two observations explain the mechanism of specificity degeneration based mainly on the effect of compensation in interaction energies of serine (P_{-2}) and phenylalanine (P_0). The remaining detailed observations regarding other aspects of PDZ domain interactions are given in [H2].

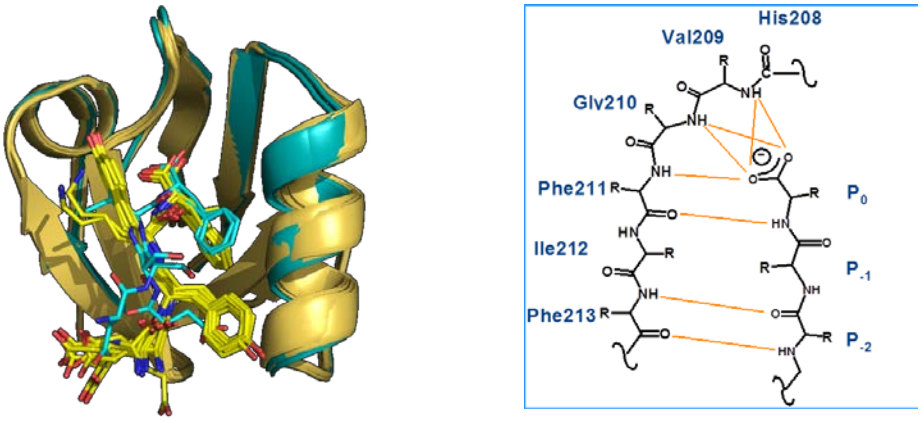

Fig. 2.7. Structural details of the complexes of the syntenin PDZ2 domain. *Left*: superposition of PDZ2 domains interacting with type I (blue) and type II (yellow) peptides. *Right*: canonical hydrogen bonds formed between the protein (left) and peptide (right). The figure is a copy of Figure 15 from the publication H2.

***Influenza* virus neuraminidase** is responsible for the release of virus from infected cells, and the transport of the virus through the mucus in the respiratory tract. It works by catalyzing the hydrolysis reaction of the glycosidic bond between the terminal sialic acid and the rest of glycoconjugates present on the surfaces of the virus and the infected cell. Despite considerable differences between the sequences of neuraminidase coming from different types and strains of influenza virus, the sialic acid-binding site is highly conserved structurally and sequentially, Fig. 2.8. Sialic acid, as a reaction product, is a native inhibitor of neuraminidase. A lot of effort has been directed at designing new neuraminidase inhibitors that could be used as drugs against influenza.

The analysis of energetic aspects of the electrostatic interaction of neuraminidase with the known inhibitors (representing more than 70 complexes of enzymes from different strains of the virus interacting with 25 different inhibitors) carried out by me showed, among other things:

- Seventeen conserved amino acid residues that build the inhibitor binding site are responsible for about 85% of the electrostatic interaction energy with the analyzed enzyme inhibitors. This justifies focusing only on these amino acid residues for the rest of the analysis.
- A correlation is observed between the electrostatic energy of conserved residues interactions, $E_{es.cons}$, and the experimentally determined strength of inhibition for the studied molecules (pK_i or p*IC50* values, Fig. 2.8). This indicates the potential for application of the method UBDB+EPMM to build a scoring function in docking procedures.
- Analysis of the contribution of each fragment of inhibitor to the interaction energy allowed for the relative ranking of the importance of various fragments and illustrated the energetic effect of the change of the substituents at a given position in the

inhibitor, for example: (a) the C2 inhibitor fragment has a dominant contribution to the interaction; changing the native carboxyl group (charge (1–)) for the phosphate group ((2–) assuming full deprotonation) significantly increases the energy of interaction; any change in another fragment of inhibitor causing worse geometrical fit of the fragment C2 to binding amino acid residues has a large effect on the interaction energy, (b) the second greatest change in the electrostatic energy induced by substituent changes is observed for position C4 and positively charged substituents (amino or guanidino groups).

- Entropic effects related to, for example, displacement of the structural water molecules with the inhibitor (differentiation between inhibitors with amino or guanidino group at position 4), or change in the number of conformational degrees of freedom when the labile inhibitors form a complex with proteins (inhibitors with the labile phosphate group at position C2) must be taken into account while constructing a proper scoring function to assess the strength of the inhibition.
- Analysis of the electrostatic interaction energy of selected structural water molecules with inhibitor and protein, made jointly with my doctoral student Katarzyna Jarzembska, allowed estimation of the relative costs of displacing some water molecules by a guanidino group at the C4 inhibitor position.
- Analysis of complexes with native protein and Arg291→Lys mutant helped to understand the electrostatic consequences of mutations as a response of the virus to drug treatment. Weakening of the electrostatic binding of the C2 inhibitor group with a mutated amino acid residue, observed by me, agrees qualitatively with the weakening of the inhibition strength of studied molecules when interacting with the mutant. Detailed analyses also indicate that the mutant virus is more resistant to the inhibitor having a hydrophobic side chain at position C6 (experimental observation) because of the electrostatic consequences of mutation.

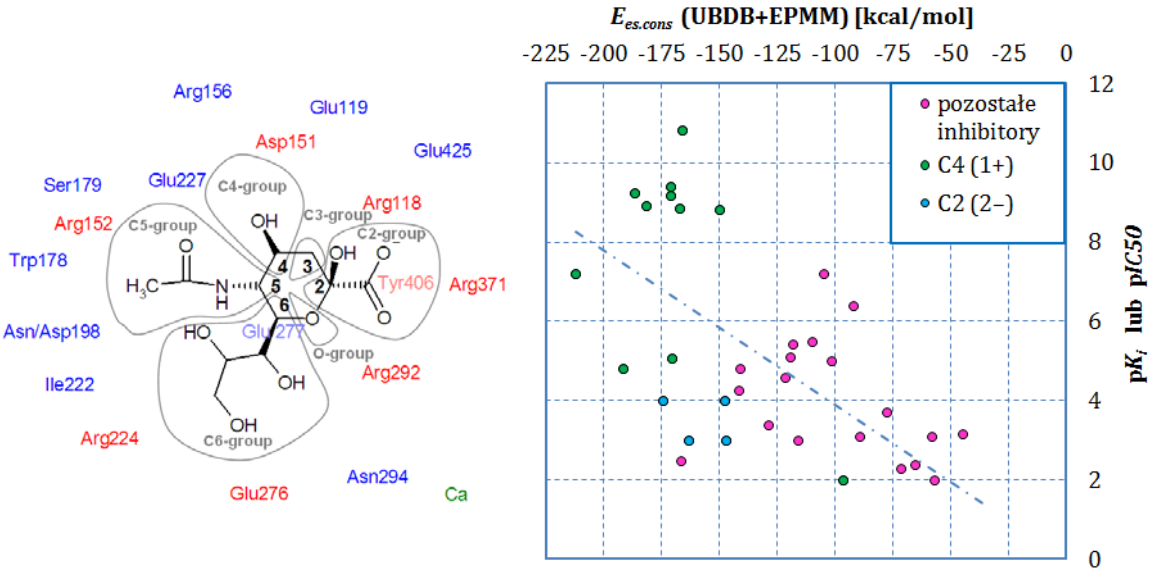

Fig. 2.8. *Left*: Schematic representation of the active site of *Influenza* virus neuraminidase and its interaction with sialic acid. The positions of conserved functional amino acid residues (red) and structural (green) are indicated. Six fragments of sialic acid are shown in grey contours. The figure is a copy of Figure 2 in the publication H3. *Right*: The correlation between the values of the electrostatic interaction energy for conserved amino acid residues interacting with the inhibitors calculated using the UBDB+EPMM method, $E_{es.cons}$ (UBDB+EPMM) [kcal/mol], and experimental values of the inhibition constant, pK_i or p*IC50*.

3. Importance for the development of the field

a. Sample Applications

The number of UBDB users is steadily growing. Many studies using UBDB are in progress; just a few have already been published [P2-P4, 28]. Those that I co-authored are shortly described below.

We used the UBDB as a source of aspherical scattering factors in TAAM refinement in order to analyze standard resolution X-ray data collected for a series of crystals of uracil derivatives [P4]. The intention of the study was to characterize the properties of the molecules, to analyze the nature of intermolecular interactions and to find a link between the molecule and the crystal architecture - issues that are important from the point of view of crystal engineering, among others. For this purpose, we carried out quantum-mechanical calculations (periodic and for isolated dimers) based on experimentally-obtained geometries. The results clearly showed how important it is to **determine** the best possible **positions of hydrogen atoms**. Cohesive energies of the crystal, for example, calculated with geometries from TAAM refinements differ on average by only 0.5 kcal/mol from the results for the optimized geometry. In the case of IAM models this difference is 3.6 kcal/mol, which is about 15% of the absolute value of the analyzed energy and does not permit a reliable quantitative analysis of the interaction energy. The results indicate that the use of TAAM refinement for polymorphs analysis, for which differences in the cohesive energy are of a few kcal/mol, would be extremely valuable.

In our next work [P3] we employed TAAM refinement to create **a starting model** for full multipole refinement of high resolution X-ray data collected for a co-crystal of 9-methyladenine with 1-methylthymine - this was the first published experimentally determined electron density of a nucleic acid base pair. For crystals of monomers constituting the above-mentioned dimer, for which we managed to collect just standard resolution data, we also conducted TAAM refinement. Obtaining the monomer geometry of a quality comparable to the geometry from multipole refinement has enabled us to compare geometric and energetic aspects of intermolecular interactions present in the analyzed crystal structures. We have obtained important results not only from the viewpoint of crystal engineering, but also for understanding the potential of the nucleic acid bases to create various types of interactions in biological systems, not just the standard Watson-Crick type.

Bank UBDB also proved to be useful in refinement of high-resolution X-ray data for 6-methyl-2thiouracyl crystal [P2]. Full multipole refinement fails to lead to a physically reliable model of density around the sulfur atom. We used therefore the UBDB to model the deformation density of the sulfur atom. This approach allowed us to test a variety of hypotheses designed to explain the presence of additional electron density peaks around the sulfur atom (anharmonic vibrations, tautomerism, oxidation). Since none of the hypotheses have been proven, in the final model the parameters of deformation density functions describing the sulfur atom were fixed at the values transferred from the UBDB, whereas the sulfur atom valence population was refined. The resulting physically correct model of the electron density of the crystal allowed us to perform a topological analysis of the interactions in the crystal lattice.

b. Summary

The results obtained by me (or under my direction) led to the development of a new method that enables the routine use of a TAAM model in refinement of X-ray diffraction data from standard-resolution measurements on single crystals. Currently, approximately 40 000 new organic crystal structures are published per year throughout the world. The quality of geometrical data obtained could be significantly improved through the use of TAAM refinement.

The method allows a rapid and satisfactory quantitative reconstruction of electron density distributions for important biological macromolecules, which so far has been difficult to achieve using quantum-mechanical methods because of the size of the system and not possible for the currently-used force fields due to excessive simplification. Also, in the case of small organic molecules, the speed of obtaining information about electronic properties of molecules can be attractive for large-scale screening of molecules with potential therapeutic properties. These applications extend far beyond the crystallography field.

In general, the developed method can be used by a wide range of scientists studying molecular crystals (design of new materials, characterization of polymorphs in pharmacology) and proteins, nucleic acids and their complexes (understanding the mechanisms of ligand recognition, rational drug design, etc.).

4. References

[H1-H8] – publications listed under I.4.b)
[P1-P33] – publications listed under III.A)
[P34] – publication listed under III.C)

[1] Hansen, N., Coppens, P.: Testing aspherical atom refinements on small-molecule datasets. Acta Cryst. A 34, 909–921 (1978)
[2] Bader, R.W.F.: Atoms in Molecules - A Quantum Theory. University of Oxford Press,Oxford (1990)
[3] Abramov Y., Volkov A., Coppens P., **1999**, **Chem. Phys. Lett**. *311*, 81–86; Bianchi R., Gatti C., Adovasio V., Nardelli M., **1996**, **Acta Crystallogr. B** *52*, 471–478; Spackman M., Byrom P., **1996**, **Acta Crystallogr. B** *52*, 1023–1035; Swaminathan S., Craven B.M., Spackman M.A., Stewart R.F., **1984**, **Acta Crystallogr., B** *40*, 398–404; Volkov A., Coppens P., **2001**, **Acta Crystallogr. A** *57*, 395–405; Volkov A., Gatti C., Abramov Y.A., Coppens P., **2000**, **Acta Crystallogr. A** *56*, 252–258.
[4] de Vries R.Y., Feil D., Tsirelson V.G., **2000**, **Acta Crystallogr. B** *56*, 118–123; Spackman M.A., Byrom P.G., Alfredsson M., Hermansson K., **1999**, **Acta Crystallogr. A** *55*, 30–47; Dittrich B., Spackman M.A., **2007**, **Acta Crystallogr. A** *63*, 426–436.
[5] Jayatilaka, D., **1998**, **Phys. Rev. Lett.** *80*, 798–801; Jayatilaka D., Grimwood D.J., **2001**, **Acta Crystallogr. A** *57 Part 1*, 76–86.
[6] Hibbs D.E., Howard S.T., Huke J.P., Waller M.P., **2005**, **Phys. Chem. Chem. Phys.** *7*, 1772–1778; Waller M.P., Howard S.T., Platts J.A., Piltz R.O., Willock D.J., Hibbs D.E., **2006**, **Chem. Eur. J.** *12*, 7603–7614.
[7] van Smaalen S., Netzel J., **2009**, **Phys. Scr.** *79*, 048304.
[8] Brock C., Dunitz J., Hirshfeld, F., **1991**, **Acta Crystallogr. B** *47*, 789–797.
[9] Pichon-Pesme V., Lecomte C., Lachekar H., **1995**, **J. Phys. Chem.** *99*, 6242–6250.
[10] Koritsanszky T., Volkov A., Coppens P., **2002**, **Acta Crystallogr. A** *58*, 464–472.
[11] Volkov A., Li, X., Koritsanszky T., Coppens P., **2004**, **J. Phys. Chem. A** *108*, 4283–4300.
[12] Dittrich B., Koritsanszky T., Luger P., **2004**, **Angew. Chem. Int. Ed. Engl.** *43*, 2718–2721.
[13] Zarychta B., Pichon-Pesme V., Guillot B., Lecomte C., Jelsch C., **2007**, **Acta Crystallogr. A** *63*, 108–125.
[14] Domagała S., Fournier B., Liebschner D., Guillot B., Jelsch C., **2012**, **Acta Crystallogr A** *68*, 337–351.

[15] Dittrich B., Hübschle C.B., Luger P., Spackman M.A., **2006**, **Acta Crystallogr. D** *62*, 1325–1335.
[16] Do 2005 roku ukazało się: Jelsch C., Pichon-Pesme V., Lecomte C., Aubry A., **1998**, **Acta Crystallogr. D** *54*, 1306–1318 ; Fernández-Serra M.V., Junquera J., Jelsch C., Lecomte C., Artacho E., **2000**, **Solid State Comm.**, *116*, 395–400; Housset D., Benabicha F., Pichon-Pesme V., Jelsch C., Maierhofer A., David S., Fontecilla-Camps J. C., Lecomte C., **2000**, **Acta Crystallogr. D** *56*, 151–160; Jelsch C., Teeter T. T., Lamzin V., Pichon-Pesme V., Blessing R. H., Lecomte C., **2000**, **Proc. Nat. Acad. Sci. USA.**, *97*, 3171–3176; Muzet N., Guillot B., Jelsch C., Lecomte C., **2003**, **Proc. Natl. Acad. Sci. USA**, *100*, 8742–8747; Schmidt A., Jelsch C., Ostergaard P., Rypniewski W., Lamzin V.S., **2003**, **J. Biol. Chem.**, *278*, 43357-43357; Pichon-Pesme V., Jelsch C., Guillot B., Lecomte C., **2004**, **Acta Crystallogr. A** *60*, 204-208; Volkov A., Koritsanszky T., Li X., Coppens P., **2004**, **Acta Crystallogr. A** *60*, 638–639; Dittrich B., Hübschle C. B., Messerschmidt M., Kalinowski R., Girnt D., Luger P., **2005**, **Acta Crystallogr. A** *61*, 314–320.
[17] Allen F. H. & Bruno I. J., **2010**, **Acta Crystallogr. B** *66*, 380–386.
[18] Koritsanszky T., Volkov A., Coppens P., **2002**, **Acta Crystallogr. A** *58*, 464–472.
[19] Hirshfeld F. L., **1977**, **Theoret. Chim. Acta**, *44*, 129–138.
[20] Koritsanszky T., Volkov A., Chodkiewicz M., **2012**, **Struct. Bond.** *47*, 1–25; Jayatilaka D., Dittrich B., **2008**, **Acta Crystallogr. A** *64*, 383–393.
[21] Volkov A., King H. F., Coppens P. **2006**, **J. Chem. Theory Comput.** *2*, 81–89.
[22] Li X., Volkov A. V., Szalewicz K., Coppens P., **2006**, **Acta Crystallogr. D** 62, 639-647.
[23] Volkov A., Koritsanszky T., Coppens P., **2004**, **Chem. Phys. Lett.** *391*, 170–175.
[24] Chalasinski G., Gutowski M., **1988**, **Chem. Rev**. *88*, 943–962.
[25] Rezac J., Riley K. E., Hobza P., **2011**, **J. Chem. Theory Comput.** *7*, 2427–2438; Jurecka P., Sponer J., Cerny J., Hobza P., **2006**, **Phys. Chem. Chem. Phys.**, *8*, 1985–1993.
[26] Bojarowski S., **2012**, „Porównanie właściwości elektrostatycznych przy użyciu banku asferycznych pseudoatomów i wybranych pól siłowych", praca magisterska, Uniwersytet Warszawski.
[27] Volkov A., Messerschmidt M., Coppens P., **2007**, **Acta Crystallogr. D** *63*, 160-170.
[28] Jarzembska K. N., Kaminski R., Wenger E., Lecomte C. & Dominiak P. M. **2013**, **J. Phys. Chem. C**, *117*, 7764-7775.

5. Discussion of the other scientific (artistic) achievements.

My other research achievements have been published in 33 publications. Among these, I consider as the most important the following:

- Improvement of the methodology used in the time-resolved diffraction studies of excited states of molecules in crystals by laser pump-X-ray probe methods. The improvement allows the estimation and elimination of temperature effects[P22].

- Characterization of the intramolecular O. .. H. .. N hydrogen bond in Schiff bases using X-ray diffraction methods, experimental measurements of the electron density distribution, statistical analysis of the structural data and the analysis of the isotope effect on the ^{13}C NMR spectrum [P26, P28, P31].

- Observation of the universal relationships among the parameters describing the chemical bonds and other interactions in the light of QTAIM theory, research based on experimental electron density distributions [P21].

- Characterization of the nature of the N…P interaction in *peri*-substituted naphthalenes using X-ray diffraction methods, statistical analysis of structural data and topological analysis of the theoretical electron density distributions [P15, P24, P33].

- Proposing the molecular mechanism for the flip-flop enzymatic action which occurs in

the family of thiamine pyrophosphate (TPP) -dependent enzymes; research based on the human pyruvate dehydrogenase structure solved and refined by me using X-ray diffraction data and on the structural analysis of the TPP-dependent enzymes [P29].

- Identification of the molecular basis of phase transitions in crystals of $(NH_4^+)_3H^+(SO_4^{2-})_2$ – the role of hydrogen bonding, research based on temperature-dependent structural studies using single crystal X-ray diffraction, neutron diffraction and solid state NMR [P30].

- Investigation of the importance of different types of amino acids for the enzymatic activity of plant UDP-glucose: solasodina and UDP-glucose: diosgenin glycosyltransferases using chemical reagents specifically modifying particular types of amino acids [P32].

II. List of publications representing scientific achievement, as referred to in Article 16 Paragraph 2 of the Act, together with declaration of the author, determining his individual contribution in their creation.

H1. Dominiak* P. M. & Coppens* P., **2006**, *Finding optimal radial-function parameters for S atoms in the Hansen–Coppens multipole model through refinement of theoretical densities*, **Acta Crystallogr**. *A62*, 224-227.
IF(2006)= 1.676
Times Cited on 21.05.2013= 13

My contribution to this work consisted of planning and performing calculations, interpreting results, writing the initial version of the manuscript and co-editing the manuscript in response to reviewers. My estimated contribution as a percentage is 80%.

H2. Dominiak* P. M., Volkov* A., Li X., Messerschmidt M. & Coppens* P., **2007**, *Theoretical Databank of Transferable Aspherical Atoms and Its Application to Electrostatic Interaction Energy Calculations of Macromolecules*. **J. Chem. Theory Comput.**, *3*, 232-247.
IF(2007)= 4.308
Times Cited on 21.05.2013= 45

My contribution to this work consisted of planning calculations (concerning both, the databank development and its applications), co-creating all necessary scripts, performing calculations, interpreting results, writing an initial draft of the manuscript, co-editing the manuscript in response to reviewers comments. My estimated contribution as a percentage is 70%.

H3. Dominiak* P. M., Volkov A., Dominiak A. P., Jarzembska K. N. & Coppens* P., **2009**, *Combining crystallographic information and an aspherical-atom data bank in the evaluation of the electrostatic interaction energy in an enzyme-substrate complex: influenza neuraminidase inhibition*. **Acta Crystallogr**. *D65*, 485-499.
IF(2009)= 2.257
Times Cited on 21.05.2013= 15

My personal contribution to this work consisted of planning calculations, co-creating all scripts necessary to perform calculations (except those related to interactions of

structural water), performing calculations (except those related to interactions of structural water), interpretation of results, writing an initial draft of the manuscript (with the exception of Chapter 5.5. Selected water molecules in the active site), to oversee the work concerning structural water interactions, managing scientific project including research described in this paper, co-editing the manuscript in response to reviewers comments. My estimated contribution as a percentage is 70%.

H4. Bąk J. M., Dominiak P. M., Wilson C. C. & Woźniak* K., **2009**, *Experimental charge-density study of paracetamol – multipole refinement in the presence of a disordered methyl group*, **Acta Crystallogr**. *A65*, 490-500.
IF(2009)= 49.93
Times Cited on 21.05.2013= 11

My personal contribution to this work consisted of overseeing the progress of work, co-planning of the type of refinements and analysis made, co-interpretation of results, managing research projects including research described in this paper, co-editing the manuscript (before sending it for publication, and in response to reviewers comments), co-editing the response to the reviews comments. My estimated contribution as a percentage is 40%.

H5. Bąk J. M., Domagała S., Hübschle C., Jelsch C., Dittrich B. & Dominiak* P. M., **2011**, *Verification of structural and electrostatic properties obtained by the use of different pseudoatom databases*, **Acta Crystallogr**. *A67*, 141-153.
IF(2011)= 2.076
Times Cited on 21.05.2013= 8

My personal contribution to this work consisted of initiating the study, overseeing the progress of work, co-planning of the types of refinements and analysis made, co-interpretation of results, managing research projects including research described in this paper, co-editing the manuscript (before sending it for publication, and in response to reviewers comments), correspondence with editor, co-editing the response to reviews comments. My estimated contribution as a percentage is 30%.

H6. Jarzembska* K. N. & Dominiak* P. M., **2012**, *New version of the theoretical databank of transferable aspherical pseudoatoms, UBDB2011-towards nucleic acid modelling*, **Acta Crystallogr**. *A68*, 139-147.
IF(2011)= 2.076
Times Cited on 21.05.2013= 4

My personal contribution to this work consisted of initiating the study, planning and overseeing research, co-interpretation of results, managing research projects including research described in this paper, manuscript editing, editing the response to reviews comments. My estimated contribution as a percentage is 30%.

H7. Bąk J. M., Czyżnikowska Z. & Dominiak* P. M., **2012**, *Is it possible to derive quantitative information on polarization of electron density from the multipolar model?*, **Acta Crystallogr**. *A68*, 705-714.
IF(2011)= 2.076
Times Cited on 21.05.2013= 0

My personal contribution to this work consisted of initiating the study, co-planning and overseeing the progress of work, co-interpretation of results, managing the research project including research described in this paper, co-editing the manuscript, co-editing the response to reviews comments. My estimated contribution as a percentage is 30%.

H8. Woińska M. & Dominiak* P. M., **2013**, *Transferability of Atomic Multipoles in Amino Acids and Peptides for Various Density Partitions*. **J. Phys. Chem. A**, *117*, 1535-1547.
IF(2011)= 2.946
Times Cited on 21.05.2013= 2

My personal contribution to this work consisted of initiating the study, planning and overseeing research, co-interpretation of results, managing the research project including research described in this paper, manuscript editing, editing the response to reviews comments. My estimated contribution as a percentage is 40%.

III. List of other (not included in the achievement mentioned in the paragraph II) published scientific papers (together with declaration of the author, determining his individual contribution in their creation) and indicators of achievements

A) Scientific papers in journals listed in the Journal Citation Reports (JRC)

After receiving the degree of doctor:

P1. Wesela-Bauman* G., Boiński T., Dominiak P., Hajmowicz H., Synoradzki L., Wierzbicki M., Woliński B., Woźniak, K. & Zawada K. **2013**, *Tartaric acid and its O-acyl derivatives. 7. Crystal structure of O-p-anisoyl-D-tartaric acid and its dimethylammonium salt trihydrate.* **J. Struct. Chem.**, *54*, 155-158.
IF(2011)= 0.586
Times Cited on 21.05.2013= 0

My contribution to this work consisted of supervising single crystal X-ray diffraction measurements (including data reduction, structure solution and refinement) for compounds A and B. My estimated contribution as a percentage is 5%.

P2. Jarzembska* K. N., Kaminski R., Wenger E., Lecomte C. & Dominiak P. M. **2013**, *The Interplay Between Charge Density Distribution, Crystal Structure Energetic Features and Crystal Morphology of 6-Methyl-2-Thiouracil*. **J. Phys. Chem. C**, *117*, 7764-7775.
IF(2011)= 4.805
Times Cited on 21.05.2013= 0

My personal contribution to this work consisted of initiating the study, overseeing the progress of work, managing research project including research described in this paper, co-interpretation of results, co-editing the manuscript, co-editing the response to reviews comments. My estimated contribution as a percentage is 20%.

P3. Jarzembska* K. N., Kubsik M., Kamiński R., Woźniak K. & Dominiak* P. M., **2012**, *From a Single Molecule to Molecular Crystal Architectures: Structural and Energetic Studies of Selected Uracil Derivatives*, **Cryst. Growth & Design**, *12*, 2508-2524.
IF(2011)= 4.720
Times Cited on 21.05.2013= 0

My personal contribution to this work consisted of initiation of the research topic, overseeing research, managing research project including research described in this paper, manuscript co-editing, co-editing the response to reviews comments. My estimated contribution as a percentage is 20%.

P4. Jarzembska* K. N. , Goral A. M., Gajda R. & Dominiak* P. M., **2012**, Hoogsteen-Watson-Crick 9-methyladenine:1-methylthymine complex: charge density study in the context of crystal engineering and nucleic acid base pairing **Cryst. Growth & Design**, *13*, 239-254
IF(2011)= 4.720
Times Cited on 21.05.2013= 2

My personal contribution to this work consisted of initiating the study, overseeing research, co-interpretation of results, managing research project including research described in this paper, manuscript co-editing, editing the response to reviews comments. My estimated contribution as a percentage is 30%.

P5. Czyżnikowska* Ż., Góra R. W., Zaleśny R., Lipkowski P. Jarzembska K. N., Dominiak P. M. & Leszczyński J. **2010**, *Structural Variability and the Nature of Intermolecular Interactions in Watson-Crick B-DNA Base Pairs*. **J. Phys. Chem. B**, *114*, 9629-9644.
IF(2010)= 3.603
Times Cited on 21.05.2013= 10

My personal contribution to this work consisted of managing research projects including research on the UBDB+EPMM method, cooperation initiation and planning comparison of the $\varepsilon_{el}^{(10)}$ energy with energy from the UBDB+EPMM method being developed in my research group, co-editing the manuscript. My estimated contribution as a percentage is 5%.

P6. Yeap* G.Y., Yam W.S., Dominiak P., Ito M. M., **2010**, *Synthesis and structural study on heterocyclic compounds 7-decanoyloxy-3-(4 '-substitutedpheny1)-4H-1-benzopyran-4-ones: Crystal structure of 7-decanoyloxy-3-(4 '-methylphenyl)-4H-1-benzopyran-4-one*. **J. Mol. Struct**., *967*, 25-33.
IF(2010)= 1.599
Times Cited on 21.05.2013= 2

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 16, writing paragraph „2.6. X-ray data collection, structure solution and refinement for compound 16”. My estimated contribution as a percentage is 10%.

P7. Hoser A. A., Dominiak P. M. & Woźniak* K., **2009**, *Towards the best model for hydrogen atoms in experimental charge density refinement*. **Acta Crystallogr.** *A65*, 300-311.
IF(2009)= 49.93
Times Cited on 21.05.2013= 26

My contribution to this work consisted of co-planning type of refinements and analysis to be done, co-nterpretation of results , co-editing the manuscript. My estimated

contribution as a percentage is 15%

P8. Grolik J., Dominiak P. M., Sieroń L., Woźniak K., Eilmes* J., **2008**, *New lacunar-type and pendant groups containing derivatives of β-unsubstituted dibenzotetraaza[14]annulenes—syntheses and crystal structures*. **Tetrahedron**, *64*, 7796-7806.
IF(2008)= 2.897
Times Cited on 21.05.2013= 5

My contribution to this work consisted of performing preliminary single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 11a, performing final single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 11b, writing structural description of compounds 11a i 11b. My estimated contribution as a percentage is 10%.

P9. Smirnov L. S., Wozniak K., Dominiak P., Loose A., Natkaniec I., Frontasyeva M. V., Pomyakushina E. V., Baranov A. I. & Dolbinina V. V., **2008**, *Refinement of the Crystal Structure of* $[Rb_x(NH_4)_{1-x}]_3H(SO_4)_2$*(x= 0.11) by Single-Crystal X-ray and Neutron Diffraction: I. Phase II at 300 K*. **Crystallogr. Reports**, *53*, 418-427.
IF(2008)= 0.481
Times Cited on 21.05.2013= 1

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound $[Rb_x(NH_4)_{1-x}]_3H(SO_4)_2$*(x= 0.11), creating fig. 1-9, co-interpretation of results. My estimated contribution as a percentage is 15%.*

P10. Galińska M., Korybut-Daszkiewicz* B., Wawrzyniak U. E., Bilewicz* R., Śledź P., Kamiński R., Dominiak P. & Woźniak* K., **2008**, *Bis- and Tris(tetraazamacrocyclic) Copper Complexes with Disulfide Linkers*. **Eur. J. Inorg. Chem**., *2008*, 2295-2301.
IF(2008)= 2.694
Times Cited on 21.05.2013= 2

My contribution to this work consisted of coordinating single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 2Cu. My estimated contribution as a percentage is 5%.

P11. Reehuis M., Wozniak K., Dominiak P., Smirnov L. S., Natkaniec I., Baranov A. I. & Dolbinina V. V., **2007**, *Refinement of the* $(NH_4)_3H(SO_4)_2$ *Crystal Structure: II. X-Ray and Neutron Single-Crystal Diffraction from Phase II at Room Temperature*. **J. Surface Investig. X-ray, Synch. and Neutron Tech**., *1*, 637-644.
IF(2007)= 0.000
Times Cited on 21.05.2013= 0

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound $(NH_4)_3H(SO_4)_2$*, creating fig. 2-4. My estimated contribution as a percentage is 10%.*

P12. Pearsal M., Gembicky* M., Dominiak P., Larsen A., Coppens P., **2007**, *Di-μ-nitrosyl-bis[(η5-pentamethylcyclopentadienyl)ruthenium(0)](Ru-Ru).* **Acta Crystallogr**. *E63*, m2596.
IF(2007)= 0.508
Times Cited on 21.05.2013= 3

My contribution to this work consisted of structure solution and refinement. My estimated contribution as a percentage is 10%.

P13. Nikolai J., Loe Ø., Dominiak P. M., Gerlitz O. O., Autschbach* J. & Davies* H. M. L., **2007**, *Mechanistic Studies of UV Assisted [4 + 2] Cycloadditions in Synthetic Efforts toward Vibsanin E.* **J. Am. Chem. Soc**., 129, 10763-10772.
IF(2007)= 7.885
Times Cited on 21.05.2013= 14

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 27. My estimated contribution as a percentage 5 %.

P14. Seifert F., Ciszak E, Korotchkina L., Golbik R., Spinka M., Dominiak P., Sidhu S., Brauer J., Patel* M. S. & Tittmann* K., **2007**, *Phosphorylation of Serine 264 Impedes Active Site Accessibility in the E1 Component of the Human Pyruvate Dehydrogenase Multienzyme Complex‡.* **Biochemistry**, *46*, 6277-6287.
IF(2007)= 3.368
Times Cited on 21.05.2013= 7

My contribution to this work consisted of protein structure refinement. My estimated contribution as a percentage is 5%.

P15. Dominiak P. M., Schiemenz G. P. & Woźniak* K., **2007**, *Statistical Analysis of Consequences of peri-Interactions in 1-Si, 8-N- (and 1-X, 8-Y-) Substituted Naphthalenes*. **Polish J. Chem**., *81*, 663-681.
IF(2007)= 0.483
Times Cited on 21.05.2013= 2

My contribution to this work consisted of structural data gathering, performing statistical analysis, interpretation of results, writing the manuscript. My estimated contribution as a percentage is 60%.

P16.Smirnov* L. S., Melnyk G., Zink N., Woźniak K., Dominiak P., Pawlukojc A., Shuvalov L. A. & Loose A., **2007**, *Refinement of Hydrogen Positions in $(NH_4)_2SeO_4$.* **J. Surface Investig. X-ray, Synch. and Neutron Tech.**, 1, 113-119.
IF(2007)= 0.000
Times Cited on 21.05.2013= 0

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound $(NH_4)_2SeO_4$, creation of fig. 4-5. My estimated contribution as a percentage is 15%.

P17.You* Y., Daniels T. S., Dominiak P. M. & Detty M. R., **2007**, *Synthesis, spectral data, and crystal structure of two novel substitution patterns in dithiaporphyrins*. **J. Porphyrins Phthalocyanines**, *11*, 1-9.
IF(2007)= 1.023
Times Cited on 21.05.2013= 2

My contribution to this work consisted of performing single crystal X-ray diffraction measurements (including data reduction, structure solution and refinement) for compounds 1b and 2, interpretation of structural data, writing chapters „X-ray structures of 1b and 2" and „X-ray data collection and refinement". My estimated contribution as a percentage is 25%.

P18.Zheng* S. –L., Gembicky M., Messerschmidt M., Dominiak P. M., & Coppens* P., **2006**, *The Effect of the Environment on Molecular Properties: Synthesis, Structure, and Photoluminescence of Cu(I) Bis(2,9-dimethyl-1,10-phenanthroline) Nanoclusters in Eight Different Supramolecular Frameworks*. **Inorg. Chem**., *45*, 9281-9289.
IF(2006)= 3.91
Times Cited on 21.05.2013= 23

My contribution to this work consisted of helping in geometrical analysis of $[Cu(dmp)_2]^+$ *cation. My estimated contribution as a percentage is 5%.*

P19.Hedley S. J., Ventura D. L., Dominiak P. M., Nygren C. L. & Davies* H. M. L., **2006**, *Investigation into Factors Influencing Stereoselectivity in the Reactions of Heterocycles with Donor-Acceptor-Substituted Rhodium Carbenoids*. **J. Org. Chem**., *71*, 5349-5356.
IF(2006)= 3.79
Times Cited on 21.05.2013= 32

My contribution to this work consisted of performing single crystal X-ray diffraction measurements (including data reduction, structure solution and refinement) for compounds 5, 9, 15 and 20. My estimated contribution as a percentage is 5 %.

P20.West-Nielsen M., Dominiak P. M., Woźniak K., Hansen* P. E., **2006**, *Strong intramolecular hydrogen bonding involving nitro- and acetyl groups. Deuterium isotope effects on chemical shifts*. **J. Mol. Struct**., *789*, 81-91.
IF(2006)= 1.495
Times Cited on 21.05.2013= 14

My contribution to this work consisted of co-performing single crystal X-ray diffraction measurements (including data reduction, structure solution and refinement) for compounds 13, 16, 21, 22, 23 and 24. My estimated contribution as a percentage is 15 %.

P21.Dominiak P. M., Makal A., Mallinson P. R., Trzcińska K., Eilmes J., Grech E., Chruszcz M., Minor* W. & Woźniak* K., **2006**, *Continua of Interactions between Pairs of Atoms in Molecular Crystals*. **Chem. Eur. J.**, *12*, 1941-1949.
IF(2006)= 5.015
Times Cited on 21.05.2013= 38

My contribution to this work consisted of performing of preliminary multipolar refinement of compounds S4 and S5, interpretation of results, writing a first draft of the manuscript and co-editing final version of manuscript. My estimated contribution as a percentage is 50%.

P22.Coppens* P., Zheng S. –L., Gembicky M., Messerschmidt M. & Dominiak P. M., **2006**, *Supramolecular solids and time-resolved diffraction*. **Cryst. Eng. Comm**., *8*, 735-741.
IF(2006)= 3.729
Times Cited on 21.05.2013= 15

My contribution to this work consisted of taking part in time resolved single crystal X-ray diffraction measurements of compunds [Cu(NH3)2]2[THPE]2·3.25H2O and HECR-2xanthone·6MeOH, co-interpretation of results. My estimated contribution as a percentage is 10%.

P23.Galan B. R., Gembicky M., Dominiak P. M., Keister* J. B. & Diver* S. T., **2005**, *Carbon Monoxide-Promoted Carbene Insertion into the Aryl Substituent of an N-Heterocyclic Carbene Ligand: Buchner Reaction in a Ruthenium Carbene Complex*. **J. Am. Chem. Soc**., *127*, 15702-15703.
IF(2025)= 7.42
Times Cited on 21.05.2013= 57

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compound 5B, creation of tab. S5-S8 and writing experimental methods part regarding the above measurement. My estimated contribution as a percentage is 10 %.

P24.Dominiak P. M., Petersen S., Schiemenz B., Schiemenz* G. P., Woźniak* K., **2005**, *peri- Interactions in naphthalenes, 13 8-Dimethylamino-naphth-1-yl carbinols as model systems for potential N → Si/P interactions*. **J. Mol. Struct**., *751*, 172-183.
IF(2005)= 1.440
Times Cited on 21.05.2013= 5

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including data reduction, structure solution and refinement) for compounds 2a/b i 2d, creating tab.1-3 and fig.1-3 and writing experimental methods part regarding the above measurement. My estimated contribution as a percentage is 20 %.

P25. Natarajan R., Savitha G., Dominiak P., Woźniak K., and Moorthy* J. N., **2005**, *Corundum, Diamond, and PtS Metal-Organic Frameworks with a Difference: Self-Assembly of a Unique Pair of 3-Connecting D_{2d}-Symmetric 3,3',5,5'-Tetrakis(4-pyridyl)bimesityl*. **Angew. Chem. Int. Ed**., *44*, 2115-2119.
IF(2005)= 9.596
Times Cited on 21.05.2013= 112

My contribution to this work consisted of performing single crystal X-ray diffraction measurement for compound 1 (including preliminary data reduction, preliminary structure solution) and compound 3 (including data reduction, structure solution and refinement). My estimated contribution as a percentage is 10%.

Before receiving the degree of doctor:

P26. Dominiak P. M., Filarowski A., Hansen P. E. & Woźniak* K., **2005**, *Factor Analysis of Deuterium Isotope Effects on ^{13}C NMR Chemical Shifts in Schiff Bases*. **Chem. Eur. J.**, *11*, 4758-4766.
IF(2005)= 4.907
Times Cited on 21.05.2013= 9

My contribution to this work consisted of interpretation of data using statistical methods, writing the manuscript. My estimated contribution as a percentage is 40%.

P27. Kołodziejski W., Woźniak K., Herold J., Dominiak P. M., Kutner* A., **2005**, *Crystal and molecular structure of 1α-hydroxylated analogs of vitamins D*. **J. Mol. Struct**., *734*, 149-155.
IF(2005)= 1.440
Times Cited on 21.05.2013= 4

My contribution to this work consisted of performing single crystal X-ray diffraction measurement (including preliminary data reduction). My estimated contribution as a percentage is 5%.

P28. Kołodziej B., Dominiak P. M., Kościelecka A., Schilf, W. Grech E., Woźniak* K., **2004**, *Neutral and ionic multiple hydrogen bonded moieties in crystal structure of a one tripodal Schiff base*. **J. Mol. Struct**., *691*, 133-139.
IF(2004)= 1.200
Times Cited on 21.05.2013= 11

My contribution to this work consisted of performing structure solution and refinement. My estimated contribution as a percentage is 10%.

P29.Ciszak* E., Korotchkina L. G., Dominiak P. M., Sidhu S. & Patel M. S., **2003**, *Structural Basis for Flip-Flop Action of Thiamin Pyrophosphate-dependent Enzymes Revealed by Human Pyruvate Dehydrogenase*. **J. Biol. Chem.**, *278*, 21240-21246.
IF(2003)= 6.482
Times Cited on 21.05.2013= 57

My contribution to this work consisted of performing protein structure solution and refinement., interpretation of results (including proposition of mechanism of flip-flop action), preparation of first version of figures. My estimated contribution as a percentage is 40%.

P30.Dominiak P. M., Herold J., Kołodziejski W. & Woźniak* K., **2003**, *H-Bonding Dependent Structures of $(NH_4^+)_3H^+(SO_4^{2-})_2$. Mechanisms of Phase Transitions*. **Inorg. Chem**., *42*, 1590-1598.
IF(2003)= 3.389
Times Cited on 21.05.2013= 18

My contribution to this work consisted of planning experiments, performing single crystal X-ray diffraction measurement (including data reduction, structure solution and

refinement), interpretation of results, writing the manuscript. My estimated contribution as a percentage is 70%.

P31.Dominiak P. M., Grech E., Barr G., Tear S., Mallinson P. & Woźniak* K., **2003**, *Neutral and Ionic Hydrogen Bonding in Schiff Bases*. **Chem. Eur. J.**, *9*, 963-970.
IF(2003)= 4.353
Times Cited on 21.05.2013= 63

My contribution to this work consisted of performing multipolar refinement of compounds, co-interpretation of results, writing manuscript. My estimated contribution as a percentage is 30%.

P32.Nawłoka P., Kalinowska M., Pączkowski C. & Wojciechowski* Z. A. **2003**, *Evidence for essential histidine and dicarboxylic amino-acid residues in the active site of UDP-glucose : solasodine glucosyltransferase from eggplant leaves*. **Acta Biochim. Polon.**, *50*, 567-572.
IF(2003)= 0.629
Times Cited on 21.05.2013= 4

My contribution to this work consisted of planning and performing all experiments, interpretation of results. My estimated contribution as a percentage is 50%.

P33.Schiemenz* G. P., Pörksen S., Dominiak P. M. & Woźniak, K., **2002**, peri-Interactions in Naphthalenes, 6. On Hypercoordination of Phosphorus in 8-Dialkylamino-naphth-1-yl Phosphonium Salts, **Z. Naturforsch.**, *57b*, 8-18.
IF(2002)= 0.774
Times Cited on 21.05.2013= 17

My contribution to this work consisted of performing single crystal X-ray diffraction measurements (including data reduction, structure solution and refinement) for compounds 5c-f and DBAN-Br, creating tab.1 i fig.6 writing experimental methods section regarding the above measurements. My estimated contribution as a percentage is 20 %.

B) Inventions and utility models and industrial products that were protected, and have been exposed to international and national exhibitions and trade fairs

NONE

C) Monographs, scientific publications in international journals or national non-stored in the database referred to in Section III A:

1. Dominiak, P. M.; Espinosa, E.; Angyan, J. G., **2012**, „*Intermolecular interaction energies from experimental charge density studies*." in **Modern Charge-Density Analysis**, Gatti, C. & Macchi, P., (ed.), Springer London, 387-433.

   My contribution to this work consisted of writing chapter 11.2 pt „Intermolecular Interaction Energies Calculated from Experimental Charge Densities" (excluding 11.2.3.1) and co-editing the manuscript. My estimated contribution as a percentage is 40%.

D) Collective studies, collection catalogues, documentation of research works, expertise works or artistic works

NONE

E) The total *impact factor* of the Journal Citation Reports list (JCR) by year of publication:

IFsum = 216,216

F) Number of citations of publications by the database Web of Science (WoS):

653 (all), 614 (without self-citations) – on 21.05.2013

G) Hirsch index according to the database Web of Science (WoS):

14– on 21.05.2013

H) Management of international and national research projects and participation in such projects

After receiving the degree of doctor:

1. *Rozwijanie banku asferycznych atomów UBDB i jego zastosowania w rentgenografii oraz w badaniach układów biomolekularnych* (eng.: *Development of an aspherical atoms databank UBDB and its use in X-ray studies and analysis of biomolecular systems*), 2012 -, ICM University of Warsaw, Principal Investigator,
   grant for supercomputing time, G50-12, 0 zł
2. *Extending the power of X-ray analysis of macromolecular crystal data*, 2011-2014, Foundation for Polish Science, Principal Investigator,
   POMOST, POMOST/2010-2/3, 649 500 zł
3. *Optymalizacja nowej metody badawczej w rentgenografii wykorzystującej bank asferycznych atomów* (eng.: *Optimization of a new method of X-ray research based on a spherical atom databank*), 2010-2012, Polish Ministry of Science and Higher Education, Principal Investigator,
   Iuventus +, IP2010 0076/70, 200 000 zł
4. *Charakterystyka oddziaływań między zasadami azotowymi nukleotydów na podstawie eksperymentalnie wyznaczonych rozkładów gęstości elektronowych*, (eng.: *Characteristics of the interaction between bases of nucleotides on the basis of the experimentally determined electron density distributions*) 2010-2013, Polish Ministry of Science and Higher Education, Principal Investigator,
   individual research grant, N N204 129138, 409 100 zł
5. *Electrostatics of Biological Macromolecules from Crystallographic Data*, 2007-2009, Foundation for Polish Science, Principal Investigator,
   POWROTY, HOM/ed2007/3, 129 750 zł
6. *Elektrostatyka makrocząsteczek biologicznych z danych krystalograficznych przy użyciu banku asferycznych atomów* (eng.: *Electrostatics of biological macromolecules from crystallographic data using an aspherical atom databank*), 2007-2008, Department of Chemistry , University of Warsaw, Principal Investigator,
   individual research grant, 120000-501/68-BW-175601, 10 000 zł

Before receiving the degree of doctor:

7. *Natura wiązania N→P w peri-podstawionych naftalenach* (eng.: *Nature of N→P binding in peri-substituted naphtalenes*) 2003-2005, Committee for Scientific Research in Poland, PhD student,
   PhD grant, 4 T09A 121 25, PI: K. Woźniak, 34 270 zł

I) International and national awards for scientific or artistic activity

1. Scholarship for outstanding young scientists, 2011-2014, Polish Ministry of Science and Higher Education.
2. Scholarship for the best doctoral students and young doctors of the University of Warsaw funded from "THE MODERN UNIVERSITY – a comprehensive support program for doctoral students and teaching staff of the University of Warsaw" project carried out in the framework of the Human Capital Operational Program, 2009-2010, University of Warsaw.
3. Article [P7] Hoser et al. Acta Crystallogr. 2009, A65, 300-311, 2009 highlighted in The IUCr Newsletter, 2009, 17(3).
4. Cover illustration from [H3] Dominiak et al. Acta Crystallogr. 2009, D65, 485-499 and article highlighted in The IUCr Newsletter, 2009, 17(2).
5. Grzegorz Białkowski Award, 2005, Society for the Promotion of Science and the Foundation for Polish Science (FNP) for the best doctoral dissertation in the field of chemistry.

J) Oral presentations at international and national conferences

After receiving the degree of doctor:

1. Dominiak P. M., **10-14.09.2012**, *Electron density and electrostatic properties of biomacromolecules from a database of pseudoatomic densities*, **Modelling and Design of Molecular Materials 2012**, Wrocław, Polska (invited lecture).
2. Dominiak P. M., **27-28.10.2009**, *Przedstawienie i zastosowania banków asferycznych atomów*, **Bruker Polska - II Spotkanie Użytkowników**, Poznań, Polska.
3. Jarzembska K. N., Galej W., Czyżnikowska Ż., Zaleśny R., Dominiak P. M., **25-27.06.2009**, *Energia oddziaływania elektrostatycznego makrocząsteczek biologicznych otrzymywana na podstawie danych krystalograficznych*, **51 Konwersatorium Krystalograficzne, III Sesja Naukowa i Warsztaty PTK**, Wrocław, Polska.
4. Dominiak P. M., Volkov A., Coppens P., **9-12.09.2007**, *Elektrostatyka makrocząsteczek biologicznych z danych krystalograficznych*, **50 Jubileuszowy Zjazd PTCh i SITPCh**, Toruń, Polska.
5. Dominiak P. M., **1-6.07.2007**, *The UBDB Aspherical-Atom Databank Designed for Charge Density Analysis of Low-Resolution Structures and Electrostatic Evaluation of Macromolecular Complexed*, **Electron Distribution & Chemical Bonding**, **Gordon Research Conference**, Mount Holyoke College, South Hadley, MA, USA (invited lecture).
6. Dominiak P. M., **13-18.08.2006**, *Electrostatic properties and macromolecular interaction energies from the theoretical databank of transferable aspherical pseudoatoms*, **Sagamore XV**, Market Bosworth, UK (invited lecture).

Before receiving the degree of doctor:

7. Dominiak P. M., Mallinson P. and Woźniak K., **12-17.05.2003**, *Neutral and ionic hydrogen bonding in Schiff bases*, **Workshop on Advanced Methods in X-ray**

Diffraction Analysis, The XD Programming Package, Buffalo, New York, USA.

8. Dominiak P. M., Ciszak E., Korotchkina L. G., Sidhu S., and Patel M. S., 28-29.11.2003, *Model działania ludzkiej dehydrogenazy pirogronianowej*, **Sesja naukowa "Czas I przestrzeń. I. Początki … wszechświata, życia, cywilizacji"**, Wydział Biologii UW, Warszawa, Polska.

IV. Achievements in education and popularization, and information on international cooperation

A) Participation in European programs and other international and national programs

NONE

B) Active participation in national and international scientific conferences

Oral presentation after receiving the degree of doctor:

1. Dominiak P. M., **10-14.09.2012**, *Electron density and electrostatic properties of biomacromolecules from a database of pseudoatomic densities*, **Modelling and Design of Molecular Materials 2012**, Wrocław, Polska (invited lecture).
2. Dominiak P. M., **27-28.10.2009**, *Przedstawienie i zastosowania banków asferycznych atomów*, **Bruker Polska - II Spotkanie Użytkowników**, Poznań, Polska.
3. Jarzembska K. N., Galej W., Czyżnikowska Ż., Zaleśny R., Dominiak P. M., **25-27.06.2009**, *Energia oddziaływania elektrostatycznego makrocząsteczek biologicznych otrzymywana na podstawie danych krystalograficznych*, **51 Konwersatorium Krystalograficzne, III Sesja Naukowa i Warsztaty PTK**, Wrocław, Polska.
4. Dominiak P. M., Volkov A., Coppens P., **9-12.09.2007**, *Elektrostatyka makrocząsteczek biologicznych z danych krystalograficznych*, **50 Jubileuszowy Zjazd PTCh i SITPCh**, Toruń, Polska.
5. Dominiak P. M., **1-6.07.2007**, *The UBDB Aspherical-Atom Databank Designed for Charge Density Analysis of Low-Resolution Structures and Electrostatic Evaluation of Macromolecular Complexed*, **Electron Distribution & Chemical Bonding**, **Gordon Research Conference**, Mount Holyoke College, South Hadley, MA, USA (invited lecture).
6. Dominiak P. M., **13-18.08.2006**, *Electrostatic properties and macromolecular interaction energies from the theoretical databank of transferable aspherical pseudoatoms*, **Sagamore XV**, Market Bosworth, UK (invited lecture).

Oral presentation before receiving the degree of doctor:

7. Dominiak P. M., Mallinson P. and Woźniak K., **12-17.05.2003**, *Neutral and ionic hydrogen bonding in Schiff bases*, **Workshop on Advanced Methods in X-ray Diffraction Analysis, The XD Programming Package**, Buffalo, New York, USA.
8. Dominiak P. M., Ciszak E., Korotchkina L. G., Sidhu S., and Patel M. S., 28-29.11.2003, *Model działania ludzkiej dehydrogenazy pirogronianowej*, **Sesja naukowa "Czas I przestrzeń. I. Początki … wszechświata, życia, cywilizacji"**, Wydział Biologii UW, Warszawa, Polska.

Poster presentation after receiving the degree of doctor:

1. Dominiak P. M., Bąk, J., Czyżnikowska Ż., **15-20.09.2012**, Deriving quantitative information on polarization of electron density from multipolar model – possible?, **European Chage Density Meeting 6**, Strbske Pleso, Slovakia.
2. Dominiak P. M., **16-19.11.2011**, Multipolar atoms for structure refinement and

electrostatic properties of macromolecules, **Multi-Pole Approach to Structural Biology Conference**, Warszawa, Polska.

3. Galej W., Jarzembska K. N., Dominiak P. M., **2-7.08.2009**, Electrostatic (Coulombic) Component of HIV-1 Protease Inhibition – Application of Aspherical Atom Databank, **Sagamore XVI**, Santa Fe, New Mexico, USA.
4. Jarzembska K. N., Dominiak P. M., Volkov, Coppens P., **26-28.06.2008**, Electrostatic interactions of selected waters in the active site of Influenza Neuraminidase – inhibitor complexes. **50 Konwersatorium Krystalograficzne, II Sesja Naukowa PTK**, Wrocław, Polska.
5. Dominiak P. M., Volkov A., Li X., Messerschmidt M., Dominiak A. P., Coppens P., **20-25.08.2006**, Macromolecular interaction energies from a theoretical databank of transferable aspherical pseudoatoms. **18th International Conference on Physical Organic Chemistry (ICPOC-18)**. Warsaw, Poland.

Poster presentation before receiving the degree of doctor:

6. Dominiak P. M., Mallinson P. and Woźniak K., **4-9.07.2004**, Neutral and Ionic Hydrogen Bonding in Schiff Bases, **Electron Distribution & Chemical Bonding, Gordon Research Conference**. Mount Holyoke College, South Hadley, MA, USA.
7. Dominiak P. M. and Woźniak K., **4-9.07.2004**, Nature of N…P Interaction in N, P-peri-Substituted Naphthalenes, **Electron Distribution & Chemical Bonding, Gordon Research Conference**. Mount Holyoke College, South Hadley, MA, USA.
8. Dominiak P. M., Filarowski A., Hansen, P. E. and Woźniak K., **15-20.02.2004**, Factor Analysis of 13C Isotope Effects in Schiff Bases, **Isotopes in Biological & Chemical Sciences, Gordon Research Conference**. Ventura, CA, USA.
9. Dominiak P. M., Ciszak E., Korotchkina L. G., Sidhu S. and Patel M. S., **15-18.09.2003**, Structural basis for flip-flop action of thiamin pyrophosphate-dependent enzymes revealed by human pyruvate dehydrogenase. **XLVI Zjazd PTCh i SITPCh**, Lublin, Polska
10. Dominiak P. M., Wozniak K., Barr G., Mallinson P., Grech E., **25-31.08.2001**, Charge Density Studies of Neutral and Ionic Hydrogen Bonds in Model Schiff Bases, **XX European Crystallographic Meeting** Kraków, Poland.
11. Dominiak P. M., Woźniak K., **25-31.08.2001**, H-Bonding Dependent Structures of $(NH_4^+)_3H^+(SO_4^{2-})_2$, **XX European Crystallographic Meeting** Kraków, Poland. (the best poster prize awarded)
12. Dominiak P. M., Wozniak K., **23.05-03.06.2001**, H-Bonding Dependent Structures of $(NH_4^+)_3H^+(SO_4^{2-})_2$. 32nd Crystallographic Course at the E. Majorana Centre, **Strength from Weakness: Structural Consequences of Weak Interactions on Molecules, Supermolecules and Crystals**, Erice, Sycylia, Włochy.
13. Nawłoka P. M., Pączkowski C., Kalinowska M., Wojciechowski Z. A., **11.2000**, An essential role of histydyl residues in substrate binding by glucosyltransferase UDP-glucose : solasodine from eggplant (Solanum melongena L.). **Zjazd Naukowy: Komórka, Organizm, Środowisko**. Wydział Biologii, UW, Warszawa, Polska.
14. Nawłoka P. M., Pączkowski C., Kalinowska M., Wojciechowski Z. A., **09.2000**, An essential role of histydyl residues in substrate binding by glucosyltransferase UDP-glucose : solasodine from eggplant (Solanum melongena L.), **XXXVI Zjazd Polskiego Towarzystwa Biochemicznego**, Poznań, Polska.

C) Participation in the organizing committee for the international and national scientific conferences

1. European Charge Density Meeting – ECDM7, 2015, Warszawa, Polska, member of the organizing committee.

D) Received awards other than those mentioned in point III – I)

NONE

E) Participation in consortia and research networks

NONE

F) Management of projects carried out in collaboration with researchers from other Polish and foreign centers, and in cooperation with business, other than those referred to in point III H)

1. *Nawiązanie współpracy Uniwersytetu Warszawskiego i Uniwersytetu w Getyndze na temat "Różne zastosowania banków asferycznych atomów" - wspólna publikacja, seminaria* (eng.: T*he cooperation of the University of Warsaw and the University of Göttingen on "Different banks use spherical atoms" - a joint publication, seminars*) 2009-2009, Foundation for Polish-German Cooperation, Dr. Birger Dittrich Group, Institute of Inorganic Chemistry, University of Göttingen,
small grant, 12331/09/GB, 5 000 zł

G) Participation in committees and editorial boards of scientific journals

NONE

H) Membership in international and national organizations and scientific societies

1. Polish Crystallographic Association, from 2010, member

I) Achievement in education and the popularization of science or art

1. XI Festival of Science - Warsaw, 29.09.2007, Lecture „Zobaczyć cząsteczki” (eng.: "Seeing the molecule") and equipment show at the Structural Research Laboratory, Department of Chemistry, University of Warsaw

J) Research tutoring for students and physicians in the course of specialization

1. Supervisor of MSc theses, from 2008, Department of Chemistry, University of Warsaw, 4 students:
   - mgr Sławomir Bojarowski, MSc degree in chemistry, „Porównanie właściwości elektrostatycznych przy użyciu banku asferycznych pseudoatomów i wybranych pól siłowych”, the 2011/2012 academic year;
   - mgr Marcin Kubsik, MSc degree in chemistry, „Wpływ podstawienia pochodnych uracylu na właściwości ich sieci krystalicznych”, the 2010/2011 academic year;
   - mgr Magdalena Woińska, MSc degree majoring in chemistry within the MISMaP, „The dependence of Transferability of Atomic Multipoles for Amino Acids and Peptides on Density Partition Method”, the 2009/2010 academic year, with honors;
   - mgr Wojciech Galej, MSc degree majoring in chemistry within the MISMaP,

„Elektrostatyczna składowa inhibicji HIV-1 proteazy. Zastosowanie bazy danych asferycznych atomów.” the 2008/2009 academic year, with honors.

2. Secondary supervisor of MSc thesis, 2002-2003, Department of Chemistry, University of Warsaw, 1 student:
   - mgr KingaTrzcińska, MSc degree in chemistry, „Analiza eksperymentalnej gęstości elektronowej w modelowej zasadzie Schiffa”, the 2002/2003 academic year; a poster on this work was awarded the 1st prize at the poster session of MSc theses at our Chemistry Departament.

3. Reviewer of MSc thesis, 2010, Department of Chemistry, University of Warsaw, 1 student:
   - mgr Marcin Stachowicz, MSc degree in chemistry, „Rentgenowskie badania strukturalne modelowych kryształów pod wysokim ciśnieniem”, the 2009/2010 academic year,

4. Teaching:
   - conducting exercises "Crystallography with the elements of group theory" (2013, BA)
   - conducting exercises "Introduction to Crystallography B" (2012, BA)
   - preparation and conducting the course (lecture + exercises) "Crystallography A' for Bioanalitics" (2010, MA)
   - preparation and conducting exercises "Crystallography - Laboratory" (2007, 2009, MA), "Specialization in Crystallography" (2007, 2009, 2012, 2013, MA), "Elements of Statistics" (2004, Center for Chemical Metrology), "Statistics and databases "(2003, 2004, BA).

K) Research tutoring for doctoral candidates as a scientific supervisor or secondary supervisor

1. Sławomir Bojarowski, since 2012, Department of Chemistry, University of Warsaw, informal scientific supervisor
2. Prashant Kumar, since 2011, Department of Chemistry, University of Warsaw, informal scientific supervisor
3. Aleksandra Elżbieta Pazio, since 2011, Department of Chemistry, University of Warsaw, informal scientific supervisor
4. Anna Maria Goral, since 2009, Department of Chemistry/ MISDoMP, University of Warsaw, informal scientific supervisor
5. Katarzyna Natalia Jarzembska, 2007-2012, Department of Chemistry, University of Warsaw, secondary supervisor
   „Extention of the aspherical pseudoatom databank towards nucleic acids and its application in structural, charge density and energy studies” (pol.: Rozszerzenie banku asferycznych pseudoatomów w kierunku kwasów nukleinowych i jego zastosowanie w badanaich struktury, energii i rozkładu gęstości elektronowej cząsteczek” , defended with honors;
6. Joanna Maria Bąk, 2007-2011, Department of Chemistry, University of Warsaw, informal scientific supervisor
   „Application of Pseudoatoms to Experimental Electron Density Refinement and Estimation of Electrostatic Properties of Molecules in the Crystalline State” (pol.:

Zastosowanie pseudoatomów do udokładniania eksperymentalnej gęstości elektronowej i oszacowania właściwości elektrostatycznych cząsteczek w stanie krystalicznym)

L) Internships in foreign or domestic research and academic centers

After receiving the degree of doctor:

1. CRM2 UMR CNRS 7036, Universite Henri Poincare, Faculte des Science et Techniques, Vandoeuvre les Nancy, France, 09.2009, visiting professor.
2. Department of Chemistry, State University of New York at Buffalo, Buffalo, NY, USA, 07.2007, visiting professor.
3. Department of Chemistry, State University of New York at Buffalo, Buffalo, NY, USA, 01.2005-12.2006, postdoctoral visit.

Before receiving the degree of doctor:

1. National Space Science Technology Center, Huntsville, AL, USA, 05-07.2003, doctoral internship
2. Structural Biology Laboratory under USRA's Microgravity Program at NASA Space Flight Center, Huntsville, AL USA, 01.-08.2002, doctoral internship

M) Expert opinion or other studies made upon request (commissioned)

BRAK

N) Participation in expert groups or competition committees

1. Recruitment committee in the TEAM project 'Self-assembly of functionalized inorganic-organic liquid crystalline hybrids for multifunctional nanomaterials' lead by prof. E. Górecka, 03.2013, selection of the best candidate for post-doc position, member

O) Reviewing national and international projects

1. SOLEIL Peer Review Committee 3 (PRC3), SYNCHROTRON SOLEIL, L'orme des Merisiers, France, 2010-2012, research proposals, ca. 500 (ca. 10 required extended review report)

P) Reviewing publications in international or national journals

1. Journal of Medicinal Chemistry, since 2012, 2 manuscripts.

2. The Journal of Physical Chemistry B, since 2010, 1 manuscript.

3. Acta Crystallographica Section B: Structural Science, since 2007, 7 manuscripts.

4. Acta Crystallographica Section C: Crystal Structure Communications, since 2011, 1 manuscript.

and books:

5. Modern Charge-Density Analysis, Gatti, C. & Macchi, P., (ed.) 2012, Springer London,

1 manuscript.

Q) Other achievements, not listed in Sections III A) - III P)

NONE