Curriculum Vitae

PERSONAL INFORMATION

Family name, First name: **Woźniak Krzysztof**

Researcher unique identifier(s) (such as ORCID, Research ID, etc. ...): 0000-0002-0277-294X

Date of birth: **24/03/1961**

Nationality: **Polish**

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Below: UW stands for the University of Warsaw

- **EDUCATION**

Since 2002 Full **professor**(in Poland professorship awarded by the President of the country)

1998 **Habilitation** "On Weak Interactions in Organic Solids" – awarded the Prime Minister Prize for the Best Habilitation, Chemistry Department, UW, Poland

1992 **PhD** "On Influence of H-Bonding on Properties of Molecules" - Promoter: Prof. Tadeusz Krygowski, Chemistry Department, UW, Poland

1986 **MSc**, Chemistry Department, UW, Poland

- **CURRENT POSITION(S)**

Since 2008 Head of **Crystallochemistry Laboratory**, Department of Chemistry, UW, Poland

Since 2010 **Professor** (professor ordinarius), Dept. of Chemistry, UW, Poland.

Since 2016 Head of **Laboratory for Structural and Biochemical Research**, UW Biological and Chemical Research Centre.

Since 10/2018 Research expert in WPD Pharmaceuticals (0.1 position)

- **PREVIOUS POSITIONS**

1986-1987 **Assistant Lecturer**

1987-1998 **Lecturer**

1998-2004 **Assistant professor**

2004-2010 **Professor** (professor extraordinary)

All positions at the Dept. of Chemistry, University of Warsaw, Poland.

- **FELLOWSHIPS AND AWARDS**

1994-1995 **Post-doc** Royal Society and Polish Academy of Sciences Fellowship (Prof. William Jones and Prof. Jack Klinowski's groups both at Chemistry Department, Cambridge University, UK)

1990 – 2005 ca. 10 study visits as research associates at the Department of Chemistry, Cambridge University and several visits to University of Wales (Dr. Sian Howard) and Glasgow University (Dr. Paul Mallinson,) + singular visits to University of Wisconsin at Milwaukee (Prof. T.L. Barr), Central Florida at Orlando (Prof. S. Seal), University of Texas at Houston (Prof. W. Priebe), research institutions at Tsukuba, Tokyo, Sendai (Japan) and several universities in Denmark and India

Ca. 20 **study visits to**: ISIS Chilton, RAL Daresbury, Saclay, Grenoble, Diamond

2007 **Visiting professor** - H. Poincare University at Nancy, France (Prof. C. Lecomte's group)

2014 **Sabbatical stay**: Chemistry Department, University of Cambridge, UK (Prof. W. Jones)

2007 **Invited participant of the 21st Solvay Conference in Chemistry (on molecular machines)** (I find this invitation to be my most prestigious scientific award so far).

Since 2015 **Elected Fellow of the ChemPubSoc Europe society** and member of a few domestic and international learned societies

06/2018 – Prof. W. Świętosławski Research Prize awarded by the Warsaw Branch of the Pol. Chem. Soc.

10/2018 – Prof. W. Świętosławski Research Prize awarded by the Department of Chemistry of UW (+ in the past years several others national and the University awards for teaching commitment and academic excellence)**; 7 poster prizes at international and domestic conferences and 4 cover pages in different journals.**

- **SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS**

2000 – 2018 **Promoter of 17 PhDs completed and another 6 currently in progress, >30 MSc theses.** Supervisor of ca. 30 postdoctoral fellows including Marie Curie Fellow Dr Maria Gorna (currently supervisor of 10 postdoctoral fellows), host of Prof. D. Haynes (Stellenbosch. SA)) during her sabbatical stay in my group (10-11/2018)

Research outcome: >350 refereed publications in learned scientific journals, more than 6050 citations, H-index =37 (Google Scholar 07/2019), >70 invited lectures in total

- **SCIENTIFIC INTERESTS**

Crystallography beyond Independent Atom Model, Hirshfeld Atom Refinement, experimental studies of charge densities in crystals of interesting organic, inorganic compounds and minerals, polymorphism and interactions in pharmaceutical substances, supramolecular compounds, catalysts, model systems with interesting weak and strong interactions (proton sponges, Schiff bases, etc), biological compounds, artificial

molecular machines. I am also very much interested in methodological aspects of X-ray scattering, electron and neutron diffractions including diffuse scattering and Pair Distribution Function analyses.

- **TEACHING ACTIVITIES**

I regularly teach (lectures and classes) crystallography and statistics (at least 210hrs/year, sometime more) at the Department of Chemistry of the University of Warsaw for last 32 years. I have regular lectures on: "Crystallography with elements of group theory", "Advanced Crystallography", "X-ray structural analysis", "Statistics and structural databases", "Challenges of modern crystallography", "Methods of structural biology", "Experimental methods of modern crystallography".

All positions at the Department of Chemistry, University of Warsaw, Poland

1986 – 1998	Assistant;
1998 – 2004	Adjunct (associate professor);
2004 – 2010	Professor (called in Poland extraordinary);
Since 2010	Professor (called in Poland ordinary professor)

- **ORGANISATION OF SCIENTIFIC MEETINGS**

2020, 2017 **Member of the International Programme Committee** of the 25th International Union of Crystallography (**IUCr**) Congress at Prague (Czech Republic) and chairman of session at the IUCR Congress at Hydarabad, India (2017)

2020 1st Joint Polish-German Crystallographic Conference replacing two annual meetings of the national crystallographic societies (Wrocław, Poland) **- initiator of this Conference** and member of joint Polish-German Organising Com.

2001, 2010, 2013, 2018 European Crystallographic Association Congresses Member of the **Programme Committee** (ECM20, Krakow, Poland, 2001), **chairman of sessions** at ECM26 (2010, Darmstadt, Germany), ECM28 (Warwick, UK, 2013), **member of the Scientific Committee** of ECM31 at Oviedo (Spain, 2018)

22/08/2018 - The chairman of the ECM31 Satellite Meeting on: "Progress in Instrumentation for X-Ray Diffraction and Cry-EM (Oviedo, Spain,)"

8 - 13 July 2018 - The International Union of Crystallography (IUCr)'s Sagamore XIX on Quantum Crystallography (Member of the Int. Advisory Com.) Halifax, Canada.

2016 **Head of the Organizing Committee** of the **7th European Charge Density Meeting**, 2016, CENT, Warszawa Poland – active attendance almost all conferences in this series (either scientific committee or presenting a lecture / communication or chairing sessions)

2011, 2016 Member of the Organising Committee of Interdisciplinary International Conferences **MULTI-POLE APPROACH TO STRUCTURAL BIOLOGY**, WARSAW, POLAND

2014 **United Nations Year of Crystallography**, 2014, **Head of the Organizing Committee**, International Symposium: „On the Past, Present and Future of Crystallographic Research in Poland"

2006 **18-th International Conference on Physical Organic Chemistry, ICPOC18**, Warszawa, Poland, Vice-chair of the Organizing Committee.

2017, 2018 **Member of the Organizing Committee of the 4-th European Crystallographic School in Warsaw**, Poland, (07.2017) and the Chairmen of the 1st conference of the University of Young Chemist, (Warsaw, 30/31 Aug. 2018) (for pupils form secondary schools in Warsaw).

Member of the Organising Committee of four "Smoleńsk Conferences" focused on explanation of the reasons of the Polish TU-154 aircraft crash close to the Smolensk Airport (Russia), Warsaw, Poland 11.2015, 10.2014, 10.2013 and on 10.2012.

- **INSTITUTIONAL RESPONSIBILITIES**

1990 – 2008 and 2013 – 2016 - Member of the Scientific Council of the Department of Chemistry, UW and its several committees (Research, Young Researchers, Recruitment).

2007-2010 – Member of the Scientific Council of the Institute of Organic Chemistry PAS, Warsaw, Poland.

2011-2016 Member of Committee for Crystallography of the Polish Academy of Sciences.

2017-2020 - Chairman of the Scientific Council of Pharmaceutical Institute, Warsaw, Poland

2017-2018 - Co-chairman and 2018-2021 – the chairman of the European Crystallographic Association Special Interest Group on Charge Spin and Momentum Densities (SIG2) presently named Quantum Crystallography.

2019 – representative of the Quantum Crystallography IUCR Commission to the International Programme Committee of the IUCR Congress in Prague (20120)

- **REVIEWING ACTIVITES**

- For more than last 20 years, I regularly referee (now ca. 1-2 ms per month, at the peak 1 per week) for major research journals in crystallography and chemistry such as: Crystal Growth and Design, Chemistry - A European Journal, CrystEngComm, Acta Cryst. A, Acta Cryst. B, Acta Cryst C, ChemComm, J. Phys. Chem. A, B i C, Dalton Trans., CrystEngComm, Inorganic Chemistry, Tetrahedron, J. Mol. Struct., Chem.

- a Eur. J., European J. Inorg. Chem., European Journal of Organic Chemistry, Dalton Trans., Physics and Chemistry of Liquids, Journal of Physical Chemistry Letters, J. Phys. Org. Chem., New Journal of Chemistry, Organic & Biomolecular Chemistry, Catalysis Today, Structural Chemistry, PCCP, RSC Advances, Green Chemistry and many others

2013 – Reviewer of the Harmonia Panel of NCN, Cracow, Poland, I was also reviewer of grant applications in other programs (Maestro, Opus, FNP) of domestic research agencies (NCN, NCBiR, FNP, KBN) and also NSF (USA).

Reviewer of: ca. 20 PhD theses,10 habilitations and professorships

2013-2017 – Regular reviewer of the Award Committee at the Institute of Physical Chemistry of the Polish

10 selected most important publications within the last 10 years.

1. M. Woińska, S. Grabowsky, P. M. Dominiak, K. Woźniak, D. Jayatilaka. *Hydrogen atoms can be located accurately and precisely by routine X-ray crystallography* **Science Advances, 2 No. 5 (2016) e1600192**

2. W. Fabiola Sanjuan-Szklarz, A. A. Hoser, M. Gutmann, A. Ø. Madsen, K. Woźniak *Yes, one can get better quality structures from routine data collections* **IUCr Journal, 3 (2016) 61-70**

3. A. A. Hoser, P. M. Dominiak, K. Woźniak *Towards the best model for hydrogen atoms in experimental charge density refinement* **Acta Crystallographica, A65 (2009) pp. 300-311 (Journal Highlight)**

4. M. Stachowicz, M. Malińska, M. Welch, J. Parafiniuk, K. Woźniak**,** *Experimental observation of charge-shift bond in fluorite CaF_2,* **Acta Crystallographica. B73 (2017) 643-653**

5. M. Malińska, K. N. Jarzembska, A. M. Goral, A. Kutner, P. M. Dominiak, K. Woźniak, *Interplay between sunitinb malate crystal packing, charge density distribution, and protein-ligand interactions in sunitinib-containing biological systems* **Acta Crystallographica, D70 (2014) 1257 -1270**

6. R. Kamiński, S. Domagała, K. N. Jarzembska, A. A. Hoser, W. F. Sanjuan-Szklarz, M. J. Gutmann, A. Makal, M. Malińska, J. M. Bąk, K. Woźniak, *Statistical analysis of multipole-model-derived structural parameters and multipole-model-derived charge-density properties from high-resolution X-ray diffraction experiments,* **Acta Crystallographica, A70 (2014) 72-91**

7. S. Domagała, K. Kość, S. W. Robinson, D. A. Haynes, K. Woźniak, *Dithiadiazolyl Radicals - Structures and Charge Densities of their Crystals and Co-Crystal,* **Crystal Growth & Design, 14 (9) (2014) pp. 4834–4848**

8. P M. Malińska, I. Fokt, W. Priebe, K. Woźniak, *Bromine atom interactions in biologically active acrylamide derivatives,* **Crystal Growth & Design**, **15 (6) (2015) 2632–2642.**

9 A. A. Hoser, Ł. Dobrzycki, M. J. Guttman, K. Woźniak, *Experimental and Theoretical Charge Density Studies of Similarities and Differences of two Polymorphs of Hydrated 1,8-Bis(dimethylamino)-naphthalene Hydrochloride (DMANH+x2Cl-xH5O2+),* **Cryst. Growth and Design, 10(12) (2010) 5092-5104**

10. M. Woinska, D. Jayatilaka, B. Dittrich, R. Flaig, P. Luger, K. Wozniak, P. M. Dominiak, S. Grabowsky, *Validation of X-ray wavefunction refinement,* **ChemPhysChem, 18 (23) (2017) 3334-3351 +** Front Cover: Validation of X-ray Wavefunction Refinement (ChemPhysChem 23/2017) Publication cover image: Volume18, Issue23, December 6, 2017, Page 3286,

Invited lectures to internationally established conferences within last 10 years

1. 2019 American Crystallographic Association Annual Meeting, July 20-24, 2019, Cincinnati, Kentucky, USA, *A Century after the Braggs – On Locating and Refining H-Atoms Using X-Rays and Neutrons,* (invited lecture)
2. 62. Scientific Congress of PTChem 2019, Warszawa, Poland, 2-6/09/2019, *Sto lat po odkryciach Braggów i Lauego – krystalografia oparta na asferycznych atomach, plenary lecture*
3. 25th Annual Meeting of Ger. Crystal. Society, Karlsruhe (Germany), 27–30/03/2017, *X-Ray Structural Analysis Century after the Braggs - On Precision and Accuracy of Structural Information, plenary*
4. Zentiva Pharmaceutical Company, 10-11 May 2017, Kabelovny 130, Prague, Czech Republic, *What modern crystallography can add to pharmaceutical research?*
5. Symposjum BCA, Sofia, Bulgaria, 05-07 October 2016, *A Century After the Braggs - Crystallography Beyond the Independent Atom Model, plenary*
6. European Charge Density Meeting 7, CENT Warsaw, Poland, 26/06-1/07/2016, *A century after the Braggs: on precision and accuracy of X-ray results,*
7. COST Action no. CM1402 Meeting, Action Title: From molecules to crystals - how do organic molecules form crystals (Crystallize), Marseille (France), 22–25/07/2015, *On Precision and Accuracy of Structural Information - Beyond Independent Atom Model,*
8. Agilent Technologies X-ray User Group Meeting; 26-27/02/2014, Oxford, UK, *Experimental charge densities - our newest examples of applications,*

9. Chemistry Department, Cambridge University, UK; 6 Oct., 2014, *X-Ray Structural Analysis Century after von Laue and the Braggs - On the Quality of Single Crystal X-Ray Results,*
10. Institut für Anorganische Chemie, Universität Göttingen, Germany, 8 July 2014, *A century after the discoveries of Max von Laue and the Braggs – On the Quality of Single Crystal X-Ray Results,*
11. 21st International Conference on the Chemistry of the Organic Solid State, St Catherine's College, Oxford, UK, 3 – 9/08/ 2013, *Dithiazyl Radicals - Structures and Charge Densities of their Crystals and Co-Crystals*
12. Agilent Users' Meeting 25-28.02.2012, Oxford, UK, *On the quality of single-crystal X-ray results*
13. International Conference on the Chemistry of the Organic Solid State, Indian Institute of Science, Bangalore, 26-30/06/2011, *On quantitative charge density studies of interactions in molecular crystals,*
12 Meeting of the ACA, New Orleans, USA 28/05/–2/06/2011, *On quantitative charge density studies of interactions in molecular crystals,* Invited lecture in the session created to honour Prof. Philip Coppens
13. Charlottesville, Department of Chemistry, University of Virginia, USA, 7/06/2011, *Quantitative charge density studies of interactions in molecular crystals,*
14 92nd Canadian Chemistry Conference of Canadian Chemical Society, Hamilton, Canada, 29/05/ - 3/06/2009, *Continua of Interactions Between Pairs of Atoms in Molecular Crystals*, Invited lecture to honour Prof. Richard Bader.

+ 8 invited lectures at domestic conferences in Poland + 6 oral communications at, among others, Gordon Conference on Crystal Engineering, IUCR Congress in Hydarabad, EuCheMS Congress at Seville, Sagamore Conference in Japan and two ECM meetings at Rovinij and Darmstadt.

Infrastructure

In 1990, when the Crystallochemistry Lab. got the first single crystal X-ray diffractometer, I organised crystallographic service mostly for different synthetic groups from Chemistry Department (UW) and from other institutions. Since 2007, I am also the head of the Structural Research Laboratory (SRL). Previously, I was coordinator of applications leading to the creation of the Structural Research Laboratory. The equipment of SRL includes: SAXS (Nanostar) and two WAXS (D8 Discover) powder X-ray diffractometers equipped with Cu anode, advanced spectrophotometers (CD spectrometers, spectrofluorimeter with TCSPC option, NSOM, FTIR Spectrometer with Raman Module, EPR Minispectrometer, XRF Spectrometer), HPLC coupled with Quadrupole Mass Spectrometer, single crystal Xray diffractometer, additional Single Crystal Rotating Anode X-Ray Diffractometer (Bruker AX Mo TXS with an Oxford Diffraction Helijet), NMR 700 MHz Spectrometer.

I am also the head of newly created Laboratory for Structural and Biochemical Research (LBSBio) just created at the Centre of Biological and Chemical Research of the University of Warsaw. It consits of a "wet" Structural Biology Lab. combined with strong X-ray structural laboratory. The X-ray equipment of this lab. consists of 3 SuperNova Single Source Rigaku Oxford Diffraction X-ray diffractometers with LT attachments for cryo-measurements and with Mo, Ag and Mo/Cu microsource X-ray anodes. In the wet lab we have crystallisation-related equipment such as protein crystallisation robots, automatic imaging system, microscopes, incubators, microincubators. The biophysics equipment includes: microscale thermophoresis system, plate reader with absorbance, fluorescence and luminescence modes with an automated pipetting module for enzymatic assays and readouts, thermal shift assays setup using RT-PCR and SEC-MALLS purification and analysis system for molecular weight determination, FPLC, Dynamic Light Scattering detector, nanospectrophotometers. Additionaly, we have TGA, DSC, nanooparticle mill and high temperature ovens for inogranic synthesis'.

Both above laboratories are independent research units, the first one within the structure of our Department of Chemistry of the University of Warsaw (SRL) and the other one within the Centre of Biological and Chemical Research of the University of Warsaw (LBSBio).

International experience

Visiting professor: France, at the CRM Lab in J. Bariol Inst., H. Poincare University at Nancy, France (Prof. C. Lecomte's group). 2007 – 1 month.

Sabbatical stay: Chemistry Department, University of Cambridge, UK (Prof. W. Jones' group), 2014 – 6 months

I gained most of my scientific experience in the 90-ties of the previous century during numerous visits to Cambridge where I stayed in groups of prof. William Jones and prof. Jack Klinowski. Additionally, I collaborated for years with: dr Sian Howard from the University of Wales at Cardiff (UK), dr Paul Mallinson from Glasgow University (UK), dr Chick Wilson from ISIS, Chilton and later from Glasgow(UK), prof. T. Barr from University Wisconsin - Milwaukee (USA), dr S. Seal from University of the Central Florida (USA) including exchange of students within NSF programme, prof. PE Hansen from Roskilde (Denmark), prof. G.

P. Schimenz from Kiel (Germany), Dr Matthias Guttmann (ISIS, Chilton, UK) and occasionally with many other western scientists.

By close collaboration I understand mutual visits and joint publications. Each of the above mentioned scientists visited my laboratory in Warsaw at least once (many of them a few times) with exception of dr C. Wilson whom I visited a few times at ISIS and who did not visit me in Warsaw. Occasionally, I also collaborated with several other people who are listed among the co-authors of my publications. However, for last ca. 15-20 years, I have concentrated on my own group in Warsaw.

Additionally, I had several short visits at teens of scientific institutions all over the world (UK, USA, India, China, Germany, France, Japan, Denmark, Czech Republic). Me and my group had >20 visits to different large scale facilities devoted to neutron, X-ray and ESCA measurements (ISIS Chilton, RAL, Grenoble, Sacley, Brookhaven, Aragonne).As a group, we also gain scientific expierience by bringing foreing scientists to our lab. We had quite a number of foreign visitors in our group in Warsaw who shared their experience and knowledge with us. This includes: Anders Madsen (Copenhagen, Denmark), Dietmar Stalke (Getynga Niemcy), B. Civalleri Torino (Italy) – visiting prof. in Warsaw; P. Mallinson (Glasgow, UK – many times); L. Farrugia (Glasgow, UK), W. Priebe (Houston, USA now long and fruitful collaboration), M. Duszek (Praque) – visiting prof. in Warsaw; M. Guttmann (ISIS Chilton, UK, a few times); L. Dobrzyńska (Louivain, Belgium) – long stays a few times – I have convinced her to return back to Poland; C. Lecomte and Ch. Jelsch (Nancy, France); B. Dittrich (Gottingen, Niemcy); prof. W. Minor (Charlottesville, USA – now affiliated professor at our Department); prof. Ph. Coppens (several times, Buffalo, USA); P. Munshi (Bangalore, Indie); R. Bader (Hamilton, Canada); R. Sutkey (Orlando, USA) - 2 months; T. Spalding and A. Velez (Orlando, USA) - 2 months; dr A. Houston (NSF, USA); P. Czubarow (Saint Gobain, USA), P-E Hansen (Roskilde, Dania); J. Klinowski (many times), W. Jones, M. Archangelskich(1 month and 1 week) – they all from Cambridge, UK, J. Henn (visiting professor for ca. 2 months, Bayrouth, Germany), G. Desiraju (Bangalore, India when he was the President of IUCR), V. Pedireddi (India), J. Overgaard (Denmark), D. Jayatilaka (Australia), A. Korliukov (Moscow,Russia) + a few more. Some of the above mentioned researchers came to Warsaw more than one time. We usually have 3-5 visits of foreign scientists per year. This year for example Prof. Delia Haynes fom Stellenbosch (South Africa) who got her edducation at Cambridge will come in October for her sabbatical stay in my group (in 2 week time she comes again to my lab.). I have also convinced Dr Wojciech Sławiński (ISIS, Chilton, UK) to return back to Poland and since this October he joins my group. Every year we have also quite a few domestic visitors from different institutions within Poland. Since October the 1st also Dr Mihails Arhangelskis (PhD from Cambridge, presently on post-doc at MCGill University in Canada is joining my group - he has got Sonata project from NCN.