Crystallographic Group

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RESEARCH PROFILE:

X-Ray and neutron diffraction on the solid state substances including variable temperature and high pressure studies, crystallography beyond Independent Atom Model, quantum crystallography, routine structural analysis, applications of crystallographic methods, thermodynamic profiling of molecular recognition, in particular, the solvent effects in the formation of guest-host complexes, crystallization and control of molecular crystal morphology, prediction of relative stability of interesting polymorphic structures, new methods of extracting thermodynamic properties from X-ray diffraction data and theoretical computations, treatment of thermal motion in X-ray diffraction data refinements, studies of solid substances exhibiting a significant level of crystalline disorder of different kinds (i.e. stacking faults, local structure of atom displacements or chemical short range order/disorder), structural studies on inhibition mechanisms of enzymes, macromolecular crystallography, pharmaceutical substances, mechanochemistry, prediction of crystal properties, variable temperature and high pressure studies of crystals and minerals, Pair Distribution Function investigations, phase transitions in crystals and minerals.

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CURRENT RESEARCH ACTIVITIES:

Presently, we conduct structural research and studies of electron density for crystals of organic and inorganic compounds. In particular, we examine crystals of compounds of pharmaceutical importance (for example vitamin D derivatives), biochemical or biochemical significance, crystals of supramolecular compounds (rotaxanes, catenanes), macrocyclic complexes of d and f electron metal ions, crystals of model compounds used for X-ray methodological research, minerals and inorganic compounds, etc).

The aim of most of our studies is to find a correlation between the internal structure of crystals and the properties of quantitative distribution of electron density in crystals on one side, and macroscopic properties of crystals (physical, chemical, pharmaceutical, biochemical, etc) including photophysical properties of organic and organometallic materials in the solid state. We are involved in development of new approaches in X-ray and neutron diffraction methods. We study the processes of crystallization of organic, inorganic and macromolecular compounds. We also investigate dynamic properties of solids, phase transitions in the solid state, and perform crystallographic and biochemical studies of macromolecules. Finally, we also study structures and photophysical properties of materials (minerals in particular) at high pressure: determine relationships between the crystal structure at high pressure and the resulting changes of photophysical properties and the mechanism of the excimer formation in the investigated compounds. In order to understand properties of functional materials we study novel materials exhibiting a significant level of crystalline disorder of different kinds (i.e. stacking faults, local structure of atom displacements or chemical short range order/disorder). Last but not least, an important part of our studies are structural studies on inhibition mechanisms of enzymes belonging to USP family, which remove ubiquitin from eukaryotic proteins.

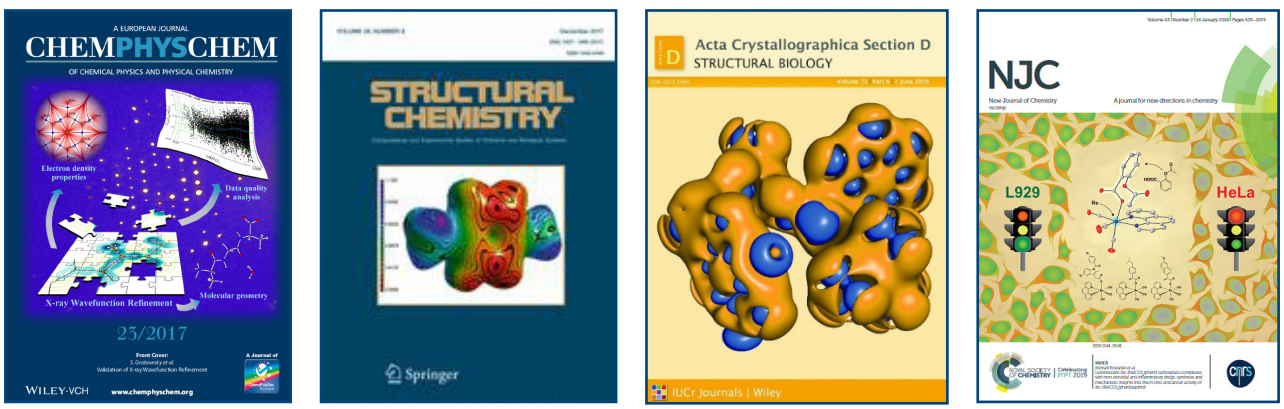

Fig. 1. (left) Front Cover: ChemPhysChem, vol 18 (2017), M. Woińska, D. Jayatilaka, B. Dittrich, R. Flaig, P. Luger, K. Woźniak, P. M. Dominiak, S. Grabowsky, Validation of X-ray Wavefunction Refinement, pp 3334 –3351, (left) Front Cover: Structural Chemistry, vol. 28, issue 6 (2017), R. Gajda, K. Woźniak, Charge density studies p-phenylenediammonium, pp. 1607–1622, (center left) Front Cover: Acta Crystallographica D, vol. 72, issue 6 (2016), M. Malinska, Z. Dauter, Transferable aspherical atom model refinement of protein and DNA structures against ultrahigh-resolution X-ray data, pp 770-779 (center right); Front Cover: J. Skiba, A. Kowalczyk, P. Stączek, T. Bernaś, D. Trzybiński, K. Woźniak, U. Schatzschneider, R. Czerwieniec, K. Kowalski, Luminescent fac-[Re(CO)3(phen)] carboxylato complexes with nonsteroidal anti-inflammatory drugs: Synthesis and mechanistic insights into the in vitro anticancer activity of fac-[Re(CO)3(phen)(aspirin)], New Journal of Chemistry, 43 (2019) 573-583 (right).

SELECTED PUBLICATIONS:

1. R. Gajda, M. Stachowicz, A. Makal, S. Sutuła, J. Parafiniuk, P. Fertay, K. Woźniak, Experimental Charge Density of Grossular Under Pressure – a Feasibility Study, IUCR J. 7(3) (2020) 383-392.
2. J.S. Mudridge, R.W. Tibble, M. Ziemniak, J. Jemielity, J.D. Gross, Structure of the activated Edc1-Dcp1-Dcp2-Edc3 mRNA decapping complex with substrate analog poised for catalysis, Nature Communications. 9(1) (2018) 1152.
3. S.W. Price, D.J. Martin, A.D. Parsons, W.A. Sławiński, A. Vamvakeros, S.J. Keylock, A.M. Beale, J.F. Mosselmans, Chemical imaging of Fischer-Tropsch catalysts under operating conditions, Science Advances. 3 (2017) 1602838.
4. S.A. Morris, G.P.M. Bignami, T. Tian, M. Navarro, D.S. Firth, J. Cejka, P.S. Wheatley, D.M. Dawson, W.A. Sławiński, D.S. Wragg, R.E. Morris, S.E. Ashbrook, In situ solid-state NMR and XRD studies of the ADOR process and the unusual structure of zeolite IPC-6, Nature Chemistry. 9(10) (2017) 1012.
5. A.A. Hoser, A.Ø. Madsen, Dynamic quantum crystallography: lattice-dynamical models refined against diffraction data. I. Theory, Acta Cryst. A72 (2016) 206–214.

6. 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(5) (2016) 1600192.
7. 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.
8. 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.
9. A.A. Hoser, P.M. Dominiak, K. Woźniak, Towards the best model for hydrogen atoms in experimental charge density refinement, Acta Crystallographica. A65 (2009) 300-311 (Journal Highlight).
10. B. Korybut-Daszkiewicz, A. Więckowska, R. Bilewicz, S. Domagała, K. Woźniak, Ellectrochemically Controlled Intramolecular Pendulum, Angewandte Chem. Int. Ed. 43 (2004) 1668–1672.