

**Experimental charge density studies:  
from organic and metal complexes to macromolecules  
Is it worth the toil?**

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# **Experimental Charge Density Studies: from organic and metal complexes to macromolecules - Is it worth the toil?**

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It is well-known that the X-ray diffraction data contain much more information than that described by the standard electron density model, used by almost (?) all refinement software. To make use of this information several methods have been proposed, of which the most popular ones are multipolar model of electron density distribution (Hansen-Coppens model) or the methods combining the experimental data with the quantum calculations. Such approaches turned out to be quite successful in the realm of small molecules, showing the importance of acquiring very good and high-resolution data. Some examples of such analyses will be presented, together with the tools used and the perspectives for further advances.

Of course, some attempts to transfer such models to the macromolecules – proteins and nucleic acids have been made, but this is quite another level of complications, caused by the lack of high-resolution data, the presence of solvent molecules, multiple conformations and by the non-centrosymmetry of the objects of the studies.

There are very few examples of (more or less) successful results which are described and the question included in the title – if these results are worth the efforts – will be addressed. Unfortunately, no ultimate answers will be presented...

## C.V.

### Maciej Kubicki

Born: January 18th, 1963, Kościan

M.Sc. in physics from Adam Mickiewicz University, 1986  
PhD: chemistry, Adam Mickiewicz University, 1991  
Habilitation: chemistry Adam Mickiewicz University, 2002.  
Professor: chemistry 2014

Currently professor at Adam Mickiewicz University;  
Dean of the Faculty of Chemistry

#### Internships:

1991-1993 University of Calgary, Calgary  
2007, 2008, 2009 University of Nancy (visiting professor)  
2016, 2017, 2018 University of Ioannina

#### Projects (PI)

0051/B/H03/2009/36 Protein structure at extreme resolution (2009 – 2011)  
UMO-2013/11/B/ST5/01681 Synthesis, structure and electron density distribution in (-)-cytisine, its salts and new derivatives - compounds of potential bioanalytical importance (2014 – 2018)  
UMO-2015/17/B/ST4/03701 Design, synthesis, X-ray structural studies and biological evaluation of novel chalcone derivatives - potential antimetabolic agents (2016 – 2020)

#### Awards

Kemula award of the Polish Chemical Society  
Zawadzki medal of the Polish Chemical Society  
Prime Minister Award  
Awards of the Rector of AMU: 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019

#### Functions

Chairman of the Poznan Division of the Polish Chemical Society  
Chairman of the Polish Crystallographic Association  
Dean of the Faculty of Chemistry

Author and coauthor of *ca.* 550 papers published in international, peer-reviewed journals  
Almost 6800 citations, Hirsch index 38 (WoS)

Some relevant publications from the last 5 years:

1. P. Žak, D. Frąckowiak, M. Grzelak, M. Bolt, M. Kubicki, B. Marciniak. *Olefin metathesis of vinylgermanium derivatives as method for the synthesis of functionalized cubic and double-decker germanosilsesquioxanes*. *Adv.Synth.Catal.* **358**, 3265-3276 (2016)
2. A. Casula, A. Llopis-Lorente, A. Garau, F. Isaia, M. Kubicki, V. Lippolis, F. Sancenón, R. Martínez-Máñez, A. Owczarzak, C. Santi, M. A. Scorciapino, C. Caltagirone. *A new class of silica-supported chromo-fluorogenic chemosensors for anion recognition based on a selenourea scaffold*.

3. K. Miłtuła, J. Duszczyk, D. Brząkałski, B. Dudziec, M. Kubicki, B. Marciniak. *Tetra-functional double-decker silsesquioxanes as anchors for reactive functional groups and potential synthons for hybrid materials*. *Chem. Commun.* **53**, 10370-10373 (2017)
4. P. Żak, M. Bolt, M. Kubicki, C. Pietraszuk. *Highly selective hydrosilylation of olefins and acetylenes by Platinum(0) complexes bearing bulky N-heterocyclic carbene ligands*. *Dalton Trans.* **47**, 1903-1910 (2018).
5. B. Orwat, M.-J. Oh, M. Kubicki, I. Kownacki. *Synthesis of 5-substituted benzo[h]quinoline derivatives via reactions involving C(sp<sup>2</sup>)-Br bond activation*. *Adv. Synth. Cat.* **360**, 3331-3344 (2018)
6. G. Dutkiewicz, E. Dutkiewicz, M. Kubicki. *Cocrystals of pyrazine and benzene polycarboxylic acids*. *Acta Cryst.* **C74**, 1420-1426 (2018).
7. P. Żak, M. Bolt, B. Dudziec, M. Kubicki. *Synthesis of (E)-1,4-disilsesquioxylsubstituted but-1-en-3-yne via Platinum-catalyzed dimerization of ethynylsiloxy-silsesquioxanes*. *Dalton Trans.* **48**, 2657-2663 (2019)
8. A. S. Hogendorf, A. Hogendorf, K. Popiołek-Barczyk, A. Ciechanowska, J. Mika, G. Satała, M. Walczak, G. Latacz, J. Handzlik, K. Kieć-Kononowicz, E. Ponimaskin, S. Schade, A. Zeug, M. Bijata, M. Kubicki, R. Kurczab, T. Lenda, J. Staroń, R. Bugno, B. Duszyńska, B. Pilarski, A. J. Bojarski. *Fluorinated indole-imidazole conjugates: Selective orally bioavailable 5-HT<sub>7</sub> receptor low-basicy agonists, potential neuropathic painkillers*. *Eur. J. Med. Chem.* **170**, 261-275 (2019).
9. K. Gholivand, M. Hosseini, Y. Maghsoud, J. Valenta, A. A. E. Valmuzi, A. Owczarzak, M. Kubicki, M. Jamshidi, M. Kahnouji. *Relations between structural and luminescence properties of novel lanthanide nitrate complexes with bis-phosphoramidate ligands*. *Inorg. Chem.* **58**, 5630-5645 (2019).
10. A. Owczarzak, Z. Dutkiewicz, R. Kurczab, W. Pietruś, M. Kubicki, A. M. Grzeńkiewicz. *Role of staple molecules in the formation of S...S contact in thioamides: experimental charge density and theoretical studies*. *Cryst. Growth Des.* **19**, 7324-7335 (2019).
11. A. M. Grzeńkiewicz, A. Ostrowska, M. Kubicki. *Solvent influence on the crystal packing of 6-aminothiocyctisine*. *Acta Cryst.* **C76**, 250-257 (2020)
12. R. Banasz, M. Kubicki, M. Wałęsa-Chorab  
*Yellow-to-brown and yellow-to-green electrochromic devices based on complexes of transition metal ions with a triphenylamine-based ligand*  
*Dalton Trans.* **49**, 15041-15053 (2020).
13. S. Napierała, M. Kubicki, M. Wałęsa-Chorab  
*Toward electrochromic metallopolymers: Synthesis and properties of polyazomethines based on complexes of transition-metal ions*  
*Inorg. Chem.* **60**, 14011-14021 (2021).
14. A. M. Grzeńkiewicz, T. Stefański, M. Kubicki  
*Weak intermolecular interactions in a series of bioactive oxazoles*  
*Molecules* **26**, 3024 (2021)