IN MEMORIAM



PROFESSOR OLEG VALER'EVICH SHISHKIN

(July 29, 1966 – July 17, 2014)

Chemistry experienced an irretrievable loss when Professor Oleg Valer'evich Shishkin died unexpectedly at age 48. Prof. Shishkin was a well-known scientist, Doctor of Chemical Sciences and Acting General Director of the State Scientific Institution "Institute for Single Crystals" of the National Academy of Sciences of Ukraine. He was a bright and unusual person.

Prof. Shishkin was born on July 29, 1966 in the village of Kolomak in Kharkov Oblast, Ukraine. He graduated with honors from secondary school in Valki, Kharkov Oblast in 1983 and from the Chemistry Faculty of Kharkov State University in 1990, having presented a thesis "Molecular and Crystal Structure of Dihydroazolopyrimidines". We should note that Prof. Shishkin devoted his whole life to the study of the molecular and crystal structure of chemical compounds and their properties.

After completing graduate study at the Organic Chemistry Faculty of Kharkov State University under the supervision of Prof. S. M. Desenko in 1993, Prof. Shishkin successfully defended his Chemical Sciences Candidate's Dissertation "Molecular Structure and Conformational Analysis of Nitrogen-containing Partially Hydrogenated Rings".

After defending his dissertation, Prof. Shishkin worked as a Senior Scientific Associate in the X-ray Structural Analysis Laboratory of the A. N. Nesmeyanov Institute of Organoelement Compounds of the Russian Academy of Sciences in Moscow from 1994 to 1997. During his stay at the Institute of Organoelement Compounds of the Russian Academy of Sciences, Prof. Shishkin completed a post-doctoral fellowship at Nottingham University in Great Britain.

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In 1997, after returning to Ukraine, Prof. Shishkin was appointed Junior Research Associate at the Institute for Single Crystals of the National Academy of Sciences of Ukraine and later, Scientific Council Secretary. Following the numerous transformations of this organization, he became Acting General Director of the State Scientific Institution "Institute for Single Crystals" of the National Academy of Sciences of Ukraine.

Prof. Shishkin defended his Doctoral Dissertation "Molecular Structure and Conformational Analysis of Six-Membered Dihydrocycles" in 1999.

Endowed with extraordinary administrative capabilities and sincere interest in research results, Prof. Shishkin was able to combine his administrative responsibilities with successful scientific work. The Department of X-ray Diffraction Studies and Quantum Chemistry, which was founded with his active participation in 1998 and led by Prof. Shishkin since its inception, is unmatched in Ukraine and recognized as one of the strongest science departments in this field in the CIS countries.

Prof. Shishkin was a respected researcher in organic, quantum, and computer chemistry. The range of his scientific interest was extraordinarily broad and encompassed current research in the molecular and crystal structure of various compounds and materials, the conformation and dynamics of organic molecules, and the analysis of intermolecular interactions in molecular complexes and crystals. He proposed a new approach to the analysis of the supramolecular architecture of molecular crystals based on a study of the topology and energetics of intermolecular interactions. Prof. Shishkin participated in joint studies with scientific institutes and universities in Ukraine, Russia, the United States, Poland, Germany, France, and other countries.

Prof. Shishkin was the author of more than one thousand scientific articles and was among the top twenty most cited Ukrainian scientists.

Prof. Shishkin attached great importance to popularizing science and appeared many times in the media, giving interviews and offering analytical articles devoted to such questions as the improvement of scientific research in today's world, on the whole, and to specific scientific advances and achievements of his research institute. Furthermore, he regarded attracting young people to science as a major challenge. Thus, he wholeheartedly supported young scientists in their research work and was an enthusiastic teacher at V. N. Karazin Kharkov National University as well as mentor of graduate students.

Prof. Shishkin will be remembered for his creative ideas, groundbreaking energy, great erudition, first-class professionalism, deep concern, and kind heartedness.

The bright memory of our beloved friend and colleague, Oleg Valer'evich Shishkin, will never leave us, giving us strength to bear the crushing blow of his loss and to prove worthy of the legacy of this remarkable man.

SOME PUBLICATIONS OF PROFESSOR O. V. SHISHKIN

- 1. S. O. Kappe, O. V. Shishkin, G. Uray, and P. Verdino, *Synthesis and reactions of Biginelli compounds*. *Part 19. Conformational analysis, entanioseparation, and determination of absolute configuration of the mitotic kinesin Eg5 inhibitor monastro, Tetrahedron*, **56**, 1859 (2000).
- 2. O. V. Shishkin, A. Pelmenschikov, D. M. Hovorun, and J. Leszczynski, *Molecular structure of free canonical 2'-deoxyribonucleosides: a density functional study, J. Mol. Struct.*, **526**, 329 (2000).
- 3. O. V. Shishkin, L. Gorb, and J. Leszczynski, *Does the hydrated cytosine molecule retain the canonical structure? A DFT study, J. Phys. Chem. B*, **104**, 5357 (2000).
- 4. O. S. Sukhanov, O. V. Shishkin, L. Gorb, Y. Podolyan, and J. Leszczynski, *Molecular structure and hydrogen bonding in polyhydrated complexes of adenine: A DFT study, J. Phys. Chem. B*, **107**, 2846 (2003).
- 5. D. S. Nesterov, V. N. Kokozay, V. V. Dyakonenko, O. V. Shishkin, J. Jezierska, A. Ozarowski, A. M. Kirillov, M. N. Kopylovich, and A. J. L. Pombeiro, *An unprecedented heterotrimetallic Fe/Cu/Co core for mild and highly efficient catalytic oxidation of cycloalkanes by hydrogen peroxide, Chem. Commun.*, 4605 (2008).

- 6. S. Shishkina, O. Shishkin, S. Desenko, and J. Leszczynski, *Conjugation and hyperconjugation in conformational analysis of cyclohexene derivatives containing an exocyclic double bond, J. Phys. Chem. A*, **112**, 7080 (2008).
- 7. O. Shishkin, Evaluation of true energy of halogen bonding in the crystals of halogen derivatives of trityl alcohol, Chem. Phys. Lett., **458**, 96 (2008).
- 8. R. Zubatyuk, O. Shishkin, L. Gorb, and J. Leszczynski, *Homonuclear versus heteronuclear resonance-assisted hydrogen bonds: tautomerism, aromaticity, and intramolecular hydrogen bonding in heterocyclic systems with different exocyclic proton donor/acceptor, J. Phys. Chem. A,* 113, 2943 (2009).
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- 10. O. Shishkin, R. Zubatyuk, V. Dyakonenko, C. Lepetit, and R. Chauvin, *The C-Cl π-interactions inside* supramolecular nanotubes of hexaethynylhexamethoxy[6]pericyclyne, Phys. Chem. Chem. Phys., **13**, 6837 (2011).
- 11. O. Shishkin, V. Dyakonenko, A. Maleev, D. Schollmeyer, and M. Vysotsky, *Columnar supramolecular architecture of crystals of 2-(4-iodophenyl)-1,10-phenanthroline derived from values of intermolecular interaction energy, CrystEngComm*, **13**, 800 (2011).
- 12. A. Furmanchuk, O. Isayev, L. Gorb, O. V. Shishkin, D. M. Hovorun, and J. Leszczynski, *Novel view on the mechanism of water-assisted proton transfer in the DNA bases: bulk water hydration, Phys. Chem. Chem. Phys.*, **13**, 4311 (2011).
- 13. O. V. Shishkin, V. V. Dyakonenko, and A. V. Maleev, *Supramolecular architecture of crystals of fused hydrocarbons based on topology of intermolecular interactions, CrystEngComm*, **14**, 1795 (2012).
- 14. O. V. Shishkin and S. V. Shishkina, *Unusual properties of usual molecules. Conformational analysis of cyclohexene, its derivatives and heterocyclic analogues*, in: J. Leszczynski and M. K. Shulka (editors), *Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends*, Springer, New York (2012), p. 557.
- 15. Oleg V. Shishkin, V. N. Medvediev, and R. I. Zubatyuk, Supramolecular architecture of molecular crystals possessing shearing mechanical properties: columns versus layers, CrystEngComm, 15, 160 (2013).
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- 17. T. A. Zubatiuk, O. V. Shishkin, L. Gorb, D. M. Hovorun, and J. Leszczynski, *B-DNA characteristics* are preserved in double stranded d(A)3-d(T)3 and d(G)3-d(C)3 minihelixes: conclusions from DFT/M06-2X study, Phys. Chem. Chem. Phys., **15**, 18155 (2013).
- 18. K. Merz, M. V. Evers, F. Uhl, R. I. Zubatyuk, and O. V. Shishkin, *Role of CHF2- and CF3-substituents* on molecular arrangement in the solid state: Experimental and theoretical crystal analysis of CH3/CHF2/CF3-substituted benzene, Cryst. Growth Des., 14, 3124 (2014).
- 19. L. Walewski, P. Dopieralski, O. V. Shishkin, and Z. Latajka, *Quantum delocalization of benzene in the ring puckering coordinates, Int. J. Quantum Chem.*, **114**, 534 (2014).
- 20. O. V. Shishkin, R. I. Zubatyuk, S. V. Shishkina, V. V. Dyakonenko, and V. V. Medvediev, *Role of supramolecular synthons in the formation of the supramolecular architecture of molecular crystals revisited from an energetic viewpoint, Phys. Chem. Chem. Phys.*, 16, 6773 (2014).

Professor, Doctor of Chemical Sciences V. A. Chebanov Professor, Doctor of Chemical Sciences S. M. Desenko SSI "Institute for Single Crystal", National Academy of Sciences of Ukraine It is difficult to overestimate the contribution of Professor Oleg Shishkin to raising the scientific level of the Chemistry of Heterocyclic Compounds. He provided thoughtful and thorough criticism as well as extremely careful and responsible editing of materials reaching this journal. Starting in 2013, Prof. Shishkin was a member of the Editorial Board. In 2014, at his initiative, a special issue of this journal (No. 3) was devoted to the application of the methods of computer chemistry in heterocyclic chemistry. He had many further ideas and plans...

We mourn with his family and colleagues.

Editorial Board and Editors of Chemistry of Heterocyclic Compounds