



Oleg Valeryevich Shishkin
(29.07.1966-17.07.2014)

Dear colleagues!

Chemical community is grieving over the tragic loss of a renowned scientist, Dr. Sc. (Chemistry), Acting General Director of the SSI "Institute for Single Crystals" of National Academy of Sciences of Ukraine, Head of Department of X-ray Diffraction Studies and Quantum Chemistry, an outstanding and most extraordinary man – Prof. Oleg Valeryevich Shishkin who passed away at the age of 47.

Prof. Oleg Shishkin was born on July 29, 1966 in Kolomak (Kharkiv Region, Ukraine). In 1983, graduated from Valki (Kharkiv Region) high school with honor, and on 1990 graduated from Kharkiv State University (Department of Chemistry) with diploma thesis dedicated to Molecular and Crystal Structure of Dihydroazolopyrimidines. Subsequently, Prof. Oleg Shishkin dedicated his entire life to the study of molecular and crystalline structure and properties of substances.

Following the completion of the PhD-course at the Department of Organic Chemistry of Kharkiv State University under the guidance of Prof. S.M. Desenko in 1993, Oleg Shishkin successfully presented thesis titled "Molecular Structure and Conformation Analysis of Nitrogenous Partially Hydrogenated Rings".

In 1994-1997, Oleg Shishkin made a career from research associate to senior researcher at the X-ray Structure Analysis Laboratory of the A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS) of Russian Academy of Sciences (Moscow). In 1995, during his tenure at the INEOS RAN, Oleg Shishkin took his fellowship at the University of Nottingham (the U.K.).

Upon the return to Ukraine in 1997, Oleg Shishkin got a job at the Institute for Single Crystals with the National Academy of Sciences of Ukraine to the position of the junior researcher, from which he proceeded to the position of academic secretary. He stayed with this organization through its numerous permutations and transformations and in 2011 he made it to the position of the Acting General Director of the SSI "Institute for Single Crystals" of National Academy of Sciences of Ukraine.

In 1999, Oleg Shishkin got his habilitation by successfully presenting thesis titled "Molecular Structure and Conformational Analysis of Hexatomic Dihydrocycles".

Exclusive organizational skills and genuine commitment to obtaining scientific results helped him combine the efficient administrative work with likewise efficient scientific activities. Founded in 1998 with active participation of and headed by Prof. Oleg Shishkin,

the Department of X-ray Diffraction Studies and Quantum Chemistry became top in Ukraine and one of the top-notch scientific groups throughout the C.I.S.

Prof. Oleg Shishkin is a renowned expert in organic, quantum and computer chemistry. His scientific interests extended to top hot problems of molecular and crystal structure of most diverse compounds and materials, study of conformational properties and dynamics of organic molecules, analysis of the character and the nature of intermolecular interaction in molecular complexes and crystals. He was the author of the innovative approach to the analysis of supramolecular architecture of molecular crystals that is based on the study of topology and the energy of intermolecular interaction. Prof. Shishkin actively cooperated with scientists representing scientific institutes and universities of Ukraine, Russia, the United States, Poland, Germany, France, etc.

As an author and co-author of over 1,000 papers, Prof. Shishkin was one of the Top-20 cited Ukrainian scientists.

Prof. Shishkin strongly believed in popularization of science, gave numerous interviews to mass media and wrote a lot of analytical articles dedicated to organizational improvement of scientific activities in contemporary conditions, giving updates on specific scientific achievements and projects of the Institution he was in charge of. In addition, he was most adamant about involvement of the youth in scientific activities and, therefore, provided strong assistance to the young researchers, enthusiastically and with ultimate commitment taught at the V.N. Karazin National University of Kharkiv and trained PhD students.

We lost a Human Being full of creative concepts, creative energy, ultimate erudite and top professional, enthusiast and a man of passion and good heart.

Fond memories of Prof. Oleg Valeryevich Shishkin – our beloved friend and colleague - will keep on inspiring us and give us strength to overcome this terrible misfortune and become worthy successors of this honorable Man.

These are some of the papers written by prof. O.V. Shishkin

1. Kappe C.O., **Shishkin O.V.**, Uray, G., Verdino P. / Synthesis and reactions of Biginelli compounds, part 19 - X-ray structure, conformational analysis, enantioseparation, and determination of absolute configuration of the mitotic kinesin Eg5 inhibitor monastrol // *TETRAHEDRON*, 2000, Vol. 56, Issue13, pp.1859-1862.
2. **Shishkin O.V.**, Pelmeshnikov A., Hovorun D.M., Leszczynski J. / Molecular structure of free canonical 2'-deoxyribonucleosides: a density functional study // *JOURNAL OF MOLECULAR STRUCTURE*, 2000, Vol. 526, pp. 329-341.
3. **Shishkin O.V.**, Gorb L., Leszczynski J. Does the hydrated cytosine molecule retain the canonical structure? A DFT study // *JOURNAL OF PHYSICAL CHEMISTRY B*, 2000, Vol. 104, Issue: 22, pp. 5357-5361.
4. Sukhanov O.S., **Shishkin O.V.**, Gorb L., Podolyan Y., Leszczynski J. / Molecular structure and hydrogen bonding in polyhydrated complexes of adenine: A DFT study // *JOURNAL OF PHYSICAL CHEMISTRY B*, 2003, Vol. 107, Issue: 12, pp. 2846-2852,
5. Nesterov D.S., Kokozay V.N., Dyakonenko V.V., **Shishkin O.V.** Jezierska J., Ozarowski A., Kirillov A.M., Kopylovich M.N., Pompeiro A.J.L. / An unprecedented heterotrimetallic Fe/Cu/Co core for mild and highly efficient catalytic oxidation of cycloalkanes by hydrogen peroxide // *CHEMICAL COMMUNICATIONS*, 2006, Issue: 44, pp. 4605-4607.
6. Shishkina S., **Shishkin O.**, Desenko S., Leszczynski J. / Conjugation and hyperconjugation in conformational analysis of cyclohexene derivatives containing an exocyclic double bond // *THE JOURNAL OF PHYSICAL CHEMISTRY, A*, 2008, 112 (30), pp. 7080-7089.
7. **Shishkin O.** / Evaluation of true energy of halogen bonding in the crystals of halogen derivatives of trityl alcohol // *CHEMICAL PHYSICS LETTERS*, 2008, 458 (1-3), pp. 96-100.
8. Zubatyuk R., **Shishkin O.**, Gorb L., Leszczynski J. // Homonuclear versus heteronuclear resonance-assisted hydrogen bonds: tautomerism, aromaticity, and intramolecular hydrogen bonding in heterocyclic systems with different exocyclic proton donor/acceptor // *THE JOURNAL OF PHYSICAL CHEMISTRY, A*, 2009, 113 (12), pp. 2943-2952.
9. Furmanchuk A., **Shishkin O.**, Isayev O., Gorb L. Leszczynski J. / New insight on structural properties of hydrated nucleic acid bases from ab initio molecular dynamics // *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 2010, 12 (33), pp. 9945-9954.
10. **Shishkin O.**, Zubatyuk R., Dyakonenko V., Lepetit C., Chauvin R. / The C-Cl π interactions inside supramolecular nanotubes of hexaethynylhexamethoxy[6]pericyclyne // *Physical chemistry chemical physics*, 2011, 13 (15), pp. 6837-6848.

11. **Shishkin O.**, Dyakonenko V., Maleev A., Schollmeyer D., Vysotsky M. / Columnar supramolecular architecture of crystals of 2-(4-Iodophenyl)-1,10-phenanthroline derived from values of intermolecular interaction energy // *CRYSTENGCOMM*, 2011, 13 (3), pp. 800-805.
12. Furmanchuk A., Isayev O., Gorb L., **Shishkin O.V.**, Hovorun D.M., Leszczynski J. / Novel view on the mechanism of water-assisted proton transfer in the DNA bases: bulk water hydration // *PHYS.CHEM.CHEM.PHYS.*, 2011, v. 13, №10, pp. 4311-4318.
13. **Shishkin O.V.**, Dyakonenko V.V., Maleev A.V. / Supramolecular architecture of crystals of fused hydrocarbons based on topology of intermolecular interactions // *CRYSTENGCOMM*, 2012, v. 14, №5, pp.1795-1794.
14. **Shishkin O.V.**, Shishkina S.V. / Unusual properties of usual molecules. Conformational analysis of cyclohexene, its derivatives and heterocyclic analogues // Eds. J. Leszczynski and M. K. Shukla. - New York: Springer, 2012. pp. 557-578.
15. **Shishkin O.V.**, Medvediev V. V., Zubatyuk R.I. / Supramolecular architecture of molecular crystals possessing shearing mechanical properties: columns versus layers // *CRYSTENGCOMM*, 2013, v. 15, №1, pp. 160-167.
16. **Shishkin O.V.**, Dopieralski P., Omelchenko I.V., Gorb L., Latajka Z., Leszczynski J / Entropy versus aromaticity in the conformational dynamics of aromatic rings // *J.MOL.MODEL.* 2013, v.19, №10, pp. 40734077.
17. Zubatiuk T.A., **Shishkin O.V.**, Gorb L., Hovorun D.M., Leszczynski J. / B-DNA characteristics are preserved in double stranded d(A)3pd(T)3 and d(G)3pd(C)3 mini-helices: conclusions from DFT/M06-2X study // *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 2013, v. 15, N 41, pp. 18155-18166.
18. Merz K., Evers M.V., Uhl F., Zubatyuk R.I., **Shishkin O.V.** / Role of CHF2- and CF3-substituents on molecular arrangement in the solid state: Experimental and theoretical crystal structure analysis of CH3/CHF2/CF3-substituted benzene // *CRYSTAL GROWTH AND DESIGN*, 2014, Vol. 14, Issue 6, pp. 3124-3130.
19. Walewski L., Dopieralski P., **Shishkin O.V.**, Latajka Z. / Quantum delocalization of benzene in the ring puckering coordinates // *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*, 2014, Vol. 114, Issue 8, pp. 534-542
20. **Shishkin O.V.**, Zubatyuk R.I., Shishkina S.V., Dyakonenko V.V., Medvediev V.V. / Role of supramolecular synthons in the formation of the supramolecular architecture of molecular crystals revisited from an energetic viewpoint // *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 2014, Vol. 16, Issue 14, pp 6773-6786.

Prof. V.A. Chebanov

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