

## ***In Memoriam: Mircea V. Diudea*** **(1950 – 2019)**

**M**IRCEA DIUDEA was a poet; in science as well in life. Poetry means transformation: to see the unseen and to transform the observation into a better flowing. Art is often regarded as the “second game”, a game beyond the natural rules or constraints, and above all – beyond entropy. To reorganize the decomposition, to rearrange the deconstruction, to recreate the reduction, to reconcile the oppositions – it is always a matter of art, with the poetry as its supremum, perhaps; and this because the poetry demands the inspiration sacrifice, the perfect verse capturing the essence of a whole story, phenomena, process, and life, sometimes a whole universe. Mircea just glimpsed to the gate of such Odeon’s mythology. Science and Art: one to one, one in one. He was basically a chemist, yet a mathematical chemical alchemist; and a good one. As good as being internationally recognized and acclaimed; sometime more ahead of his time, sometime not coping with the system, yet always flowing aside with his concepts, nano-structures, polynomials, verses and poems – articles, lessons, meetings, overworking nights, friendship, spiritualized love.

In common life terms, professor Mircea V. Diudea was born in 1950, November, 11, in Silivas, a village of Transylvania, Romania, in a family of primary school teachers. He followed the high school “Nicolae Balcescu”, Cluj and next the Faculty of Chemistry, University of Cluj (1969–1974). The PhD thesis, entitled “Phenothiazines and related structures”, performed in organic synthesis, under the guiding of two bright Chemists, Professors Valer Farcasan and Cornel Bodea, was defended in 1979, at the Institute of Chemistry, Cluj. He worked six years (1974–1980) as a chemist at “Terapia” Drug Factory-Cluj and the next seven years (1980–1987) as researcher, at Chemical-



Prof. Dr. Mircea V. Diudea

Pharmaceutical Research Institute, Cluj. From 1987 was admitted at the Faculty of Chemistry and Chemical Engineering, of “Babes-Bolyai” University, Cluj, as assistant professor (1987–1990), turned then to associate professor (1990–1996) and from 1996 to full professor, at the Department of Organic Chemistry, while chairing the main courses in Organic Chemistry and Biologically Active Compounds, along advanced courses in Molecular Topology, QSAR/QSPR, Fullerenes and Nanostructures, basically at Master and PhD levels with 18 PhD theses defended by 2016.

In 1986 he established the TOPO GROUP CLUJ, and in 2007 founded the European Society of Mathematical Chemistry ESMC, of which first president acted as such. The scientific activity in his group was supported by a dozen of original software programs. These data include a period of more than 30 years when a new interdisciplinary science,

called Molecular Topology, has been developed under his guidance and resulted in publication of more than 300 scientific articles, acquired an Hirsch index of 34 (in ISI database), with more than 3,000 citations in ISI journals and tens of authored or edited books and chapters;

Yet, Mircea's main scientific heritage was in reversely understanding the molecule – he always said “*one was the quest from structure to properties of molecules – the future will be from molecular graphs to molecular synthesis!*” What prof. Diudea anticipated is nothing than the artificial chemistry, which will be for sure a special branch for artificial intelligence age, just entering within it. Accordingly, he had tackled such long term project developing, contributing and challenging three main directions of research; they may be resumed with fundamental contributions as are:

- **In molecular topology** developed within the basic theory, with the main results including matrices (Cluj, shell, combinatorial, matriceal operators), topological indices (Cluj, Cluj-Ilmenau, Cluj-Tehran, super-index Cluj-Niš, index of centrality, centric connectivity index, etc.) and algorithms for inter and intra-molecular ordering, topological symmetry/equivalence classes of sub-graphs, for enumerating the Kekulé valence structures.
- **In QSAR/QSPR** contributed with data reduction procedures, clustering procedures based on 2D and 3D similarity, optimal regression procedures, modelling various physico-chemical properties and biological activities, including new algorithms for 2D and 3D similarity and drug design.
- **In nanoscience** he challenged the basic theory with: designing of nanostructures by operations on maps and nets, the Romanian “Capra” being the first prochiral basic operation, rules of stability of fullerenes, a modified Euler theorem in multi-shell nanostructures, original counting polynomials Omega, Pi, Theta, Cluj, design of the new diamond D<sub>5</sub> that hopefully will be produced in the NanoLab of Carbon Allotropes, organized following the legacy of his guidance, along an astonishing Gallery of molecular art, etc.

Professor Mircea Diudea was a passionate member of International Academy of Mathematical Chemistry (2005) and member of Editorial Board of: *Croatica Chemica Acta*, *MATCH Communications in Mathematical and in Computer Chemistry*, *Internet Electronic Journal of Molecular Design*, *Carpathian Journal of Mathematics*, *Iranian Journal of Mathematical Chemistry*, *Acta Universitas Cibiniensis* and Senior Editor at *International Journal of Chemical Modeling*, NOVA Publishers, New York, USA. Also he was a referee at preeminent journals in the mathematical- and physical-chemical fields, e.g., *Chem. Phys. Lett.*, *Int. Elect. J. Mol.*

*Design*, *New J. Chem.*, *SAR/QSAR Env. Res.*, *Bioorg. Med. Chem. Lett.*, *MATCH Commun. Math. Comput. Chem.*, *Fullerenes, Nanotubes Carbon Nanostruct.*, *Molecules*, *J. Am. Chem. Soc.*, *Romanian Chemical Quarterly Reviews*, *Ars Combinatorica*, *Arxivoc*, *Utilitas Math*, *Eur. J. Operational Res.*, *Math. Comput. Model.*, *J. Math. Chem.*

Within numerous international stages, collaborations, invited lectures and conferences spanning Russian Academy, Ruđer Bošković Institute at Zagreb, Central Chemical Research Institute of Hungarian Academy, DAAD fellowships at University of Bayreuth and University of Bielefeld, University of Exeter, University of Tsukuba, University of Hiroshima, University of Milano-Bicocca, University of Kashan, Tarbiat Modares University of Tehran, and many others, Professor Diudea established himself and his group as main flag in contemporary worldwide recognized Romanian molecular topology, molecular design, and design of nanostructures.

*Where to start then/Among the mute spaces/On no-walked road; Among the planets/Waved in theorems/ Difficult to prove; Dual of shadow/Seduced by the charm/Of a curved time!* (M. Diudea in his own translation, *Songs of Love*, Dellart Publishing House, Cluj-Napoca, 2012; <Unde să pornești/Where to start then>).

And the time had again no patience... this time... it was Mircea Diudea!

In the behalf of Editors, Contributors and Audience of *Croatica Chemica Acta*, we wish Prof. Mircea Diudea, a respectful Rest in Peace Dear Friend! While leaving your scientific and poetry prolong your life river!

Hearty Yours All!

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