



## PROFESSOR ALEXANDRU T. BALABAN'S 80<sup>th</sup> ANNIVERSARY



The Editorial Board of *Revue Roumaine de Chimie* continues the traditional dedication of a special issue for Professor A. T. Balaban's anniversary, in line with two previous occasions (60<sup>th</sup> and 70<sup>th</sup> anniversaries): *Rev. Roum. Chim.*, 1991, 36, 281-311 and 2001, 46, 261-275. As it was done in these issues, the list of publications continues, with a few unavoidable overlaps for publications that were misnumbered.

**Didactic and organizational activities.** After retiring from the Polytechnic University of Bucharest in 2000 and becoming a tenured professor at the Texas A&M University in Galveston (TAMUG), Department of Marine Sciences, USA, Professor A. T. Balaban taught between 1991 and 2011 one-semester courses (Organic Chemistry I and II, as well as Fundamentals of Chemistry I and II) with the exception of a sabbatical leave for the Fall Semester of 2007. In 2010 a new Science Building was inaugurated for TAMUG.

Together with a few other mathematical chemists, he founded in 2005 the *International Academy of Mathematical Chemistry*, whose first President he became for a duration of three years. The official location is in Dubrovnik, Croatia, and at present there are 81 members from 22 countries. Every year in June there is a meeting of IAMC (so far in Croatia, Slovenia, Italy) with lectures and election of a few new members.

In 2001 the Hungarian Academy of Sciences elected Professor Balaban as an Honorary Member. In 2007, the Association of Former Students of the Texas A&M University presented to Professor Balaban their annual Distinguished Achievement Award for Research (by an interesting coincidence, another awardee in the same year also originated from Roumania, Dr. Ciprian Foiaş, Professor of Mathematics).

As a member in the editorial boards of several journals, Professor Balaban spends a considerable time in refereeing manuscripts prior to publication. He is at present regional editor for *Polycyclic Aromatic Compounds* (Taylor and Francis, Publ.); Associate Editor for *Current Organic Synthesis* (Bentham Publ.); Editorial Board member for the following journals: *The Open Chemical Physics Journal*; *The Open*

*Information Science Journal; The Open Applied Informatics Journal; Current Computer-Aided Drug Design; Current Bioactive Compounds* (all from Bentham Publ.); *Advances in Heterocyclic Chemistry*, USA; *Fullerene Science and Technology*, USA; *Organic Preparations and Procedures International*, USA; *MATCH, Communications in Mathematical and Computational Chemistry*, Serbia; *Journal of Radioanalytical and Nuclear Chemistry*, Holland; *Heterocyclic Communications*, England; *Scientometrics*, Hungary; *Structural Chemistry* (Springer Publ.); *Central European Journal of Chemistry*, Poland; *Internet Electronic Journal of Molecular Modeling* (USA); *Revista de Chimie Bucureşti*, Roumania; *Revue Roumaine de Chimie*, Roumania. Previously, he was a member in the editorial boards of *Journal of Chemical Information and Computer Sciences*, USA; *Journal of Labelled Compounds and Radiopharmaceuticals*, USA; *Journal of Computational Chemistry*, USA; *Journal of Mathematical Chemistry*, Canada; *SAR and QSAR in Environmental Research*, France; *Bulletin des Sociétés Chimiques Belges*, Belgium; *Acta Chemica Hungarica – Models in Chemistry*, Hungary; and *Roumanian Chemical Quarterly Reviews*.

**Scientific research.** In **experimental chemistry**, with his former Ph. D. student in Bucharest, Marc Antoniu Ilies (who is now an Assistant Professor at the Temple University in Philadelphia), and several coworkers from TAMUG, Professor Balaban applied the Balaban-Nenitzescu-Praill reaction to the synthesis of pyrylium salts with long hydrophobic substituents. These compounds can be easily converted into pyridinium cationic lipids which self-aggregate into liposomes that can carry polynucleotides across biological membranes. A US patent was issued and several articles were published describing this new class of gene-transfer agents. Similar synthetic research is being carried out at the Center for Organic Chemistry of the Roumanian Academy in Bucharest. Another application of this reaction has led to the synthesis of new ionic liquids derived from pyrylium and pyridinium salts. On demand from the editor of the *Encyclopedia of Reagents for Organic Synthesis*, a few monographs on pyrylium salts have been included both in the printed and the electronic version. A comprehensive review of methods for preparing pyrylium salts was published by Balaban Senior (A. T.) and Junior (Teodor-Silviu) in *Science of Synthesis; Houben-Weyl Methods of Molecular Transformations* (with an up-date to appear in 2011). An experimental example of double Janus-effect was obtained with 4-ethyl-2,6-diisopropylpyridine, where the buttressing of isopropyl groups causes them to behave like *tert*-butyl groups reducing substantially the basicity of this pyridine; 2,6-diisopropylpyrylium salts and the corresponding pyridinium derivatives have interesting biological applications due to their fluorescence. Biomedical applications of such heterocyclic cations have been discovered in collaborations with Professor Claudiu Supuran, a well-known authority on carbonic anhydrase. New ionic liquids based on pyrylium and pyridinium cations were synthesized.

In collaboration with Dr. Titus Constantinescu and his coworkers from the Institute of Physical Chemistry of the Roumanian Academy in Bucharest, Professor Balaban has published several papers on the synthesis of new stable free radicals, new metal complexes involving macrocyclic polyethers, and new fluorescent compounds. This collaboration continues even after Dr. Constantinescu's retirement. In-depth investigation of fluorescent properties have benefitted from collaborations with Professor Mihaela Hillebrand from the Bucharest University and her Ph. D. students.

In **theoretical chemistry**, Professor Balaban has authored two book chapters on the aromaticity of heterocycles. In collaboration with Professor Katritzky and Dr. Daniela Oniciu, Dr. Balaban has published a review about "aromaticity as a cornerstone in heterocyclic chemistry". Other reviews worthy of mention are a chapter on nanocones in a book edited by Mircea Diudea, and a chapter on molecular descriptors in drug design published in *Encyclopedia of Complexity and Systems Science*. In a paper published in 2006, the complexity of graphs was analyzed in terms of size, branching, and centricity. Some reflections about mathematical chemistry were published in 2005. Together with Professor D. J. Klein, the central place of chemistry in relationship with other disciplines was critically assessed.

Continuing the collaboration with Professor D. J. Klein from TAMUG, involving often also Dr. Ovidiu Ivanciu, his former Ph. D. student in Bucharest, Professor Balaban has published several papers on fullerenes, nanocones, and nanotubes. The most numerous collaborations – publications – have been with Professor Milan Randić, who became interested in graph-theoretical problems after having listened to a lecture presented by Professor Balaban in 1975 at Harvard University, and who was Vice-President of the *International Academy of Mathematical Chemistry* in 2005-2008. They published a series of six papers on the partitioning of  $\pi$ -electrons in rings of polycyclic conjugated hydrocarbons; this sharing of  $\pi$ -electrons accounts for several

characteristics of such compounds and correlates well with Eric Clar's theory. Also with Professor Randić and three other collaborators, an ample review on "graphical representations of proteins" was published in *Chemical Reviews* in 2011.

Benzeneoids that have only "Clar sextets" and "empty rings" have been characterized by Professors Balaban, Klein, and Schmalz from TAMUG as "claromatics". Also in collaboration with Professor Randić several publications have concentrated on graph-theoretical analysis of biological networks and biomolecules.

During the last few years, Professor Emeritus Norman H. March, who chaired the Department of Theoretical Chemistry of Oxford University between 1977 and 1994, visited TAMUG for one month; several collaborations with him and Professor D.J. Klein involved theoretical analyses of ionic liquids, phase transitions, and the "wetting index" of liquids.

Among topological indices (TIs) useful for quantitative structure-property relationships, the Balaban index  $J$  has several unique properties, including high discrimination ability among isomeric structures. Several studies revealed how alkanes are ordered by various TIs, relationships among TIs which can be clustered accordingly, and correlations with the structure of polycyclic benzenoid hydrocarbons.

An interesting development has occurred with Professor Balaban's conjectured *trivalent cages* (minimal regular graphs of degree three with smallest circuits involving  $g$  vertices). Mathematicians have described  $g$ -cages with  $g = 3, 4, 5, 6, 7, 8$ , and 12; the 5-cage with 10 vertices (called the Petersen graph) plays an important role in graph theory, and happens to represent a particular case of "reaction graphs" introduced by Professor Balaban in 1966. Having tried to find solutions to the unknown cases with  $g = 9, 10$ , and 11, he dared to publish conjectures on these cases. By an extremely hard and long computer search, it was proved that the conjectured 11-cage (known as Balaban's 11-cage) is unique, whereas there are exactly three 10-cages, the first of which is known as Balaban's 10-cage, and is on the cover of the book by N. Hartsfield and G. Ringel, *Pearls in Graph Theory: A Comprehensive Introduction*, Academic Press, San Diego, 1990.

An index of scientific productivity, measuring both the number of publications in peer-reviewed journals and the number of citations per publication, was introduced by A. Hirsch: the  $h$ -index is the number  $h$  of articles each of which has been cited by others at least  $h$  times. The *Web of Science* (an online academic citation index provided by Thomson Reuters), which allows easy access to citations, lists Professor Balaban's  $h$ -index as 49 (in December 2010), and provides charts for the numbers of papers and citations per year. Figs. 1 and 2 (from Thomson Reuters) illustrate yearly plots of publications and citations, respectively. The paper from *Chemical Physics Letters* that introduced index  $J$  has been cited more than 600 times.

**Published Items in Each Year**

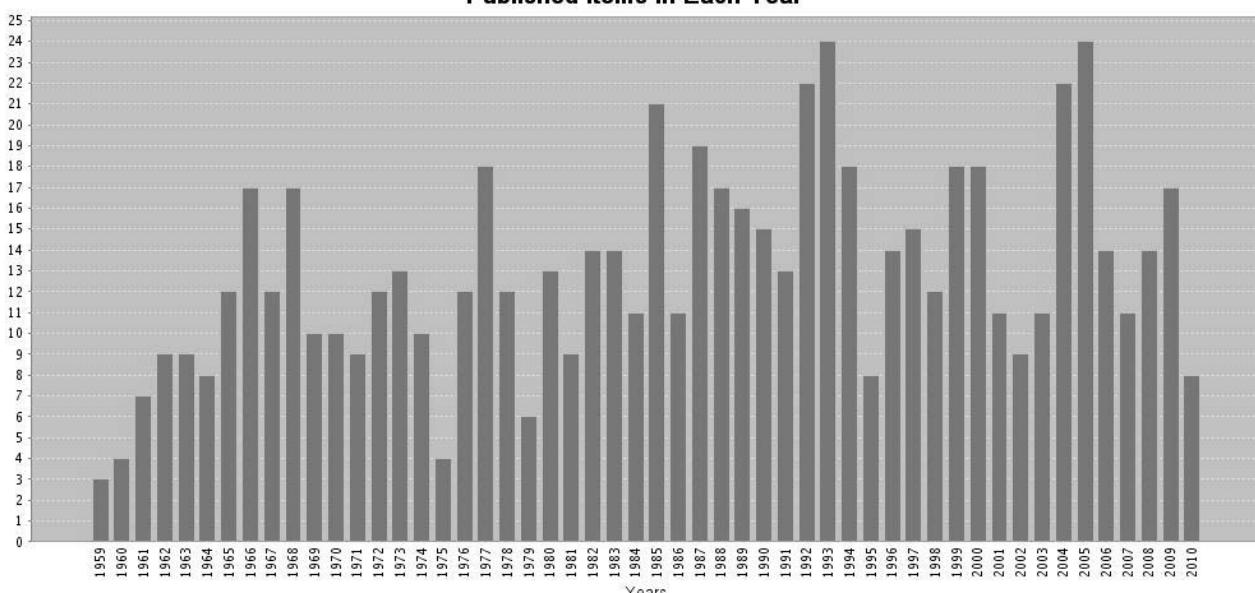


Fig. 1 – Numbers of papers published yearly by A. T. Balaban in peer-reviewed journals from 1959 till mid-2010.

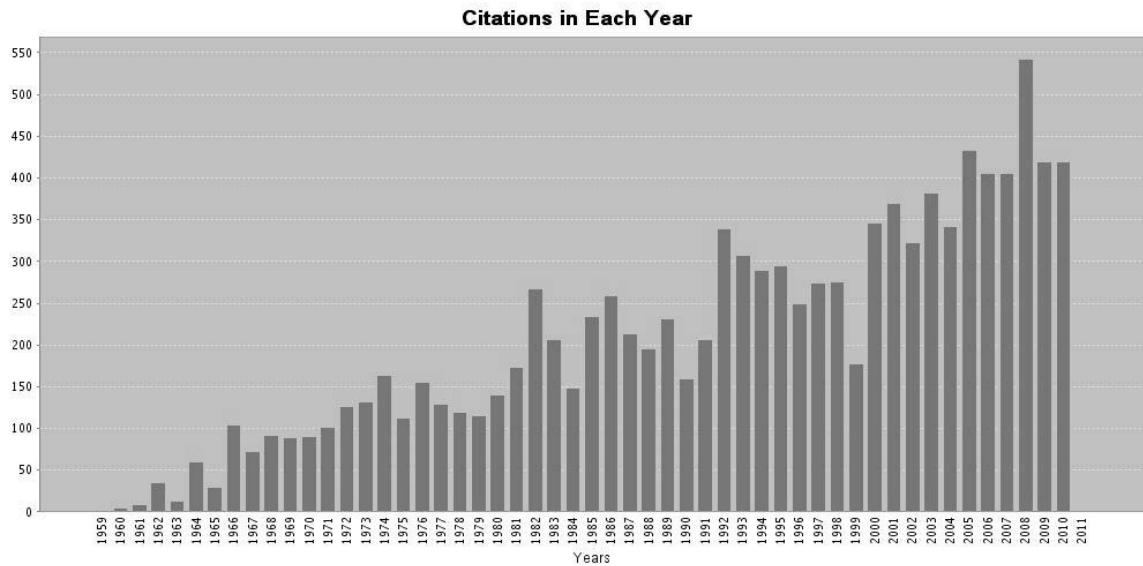


Fig. 2 – Numbers of yearly citations for A. T. Balaban’s papers between 1960 and mid-2010.

## SCIENTIFIC PUBLICATIONS OF ALEXANDRU T. BALABAN

### A. Books

#### A. 1. Edited Books

8. A.T. Balaban and C. Balaban (coordinating authors), "Small Encyclopedia of Chemical Technology" (in Roumanian), two volumes, Editura Zecasin, Bucharest, 1999-2000, 434 and 450 p.

### B. Book Chapters

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### C . Articles in peer-reviewed scientific periodicals

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#### D. Patents

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