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Parents: Teodor Balaban (electromechanical engineer), Florica Balaban (teacher)

Family: Married since 1955 to Cornelia Balaban (1929-2016, chemical engineer, Ph. D., she was a fellow student during 1949-1953, taught Chemical Engineering at the Bucharest Polytechnic University). Teodor Silviu Balaban (1958-2016, son, Ph. D., Full Professor at the University Aix-Marseille III, Chair of Supramolecular Organic Assemblies, Marseille, France) and Irina Alexandra Buhimschi (daughter, M. D., Director of the Center for Perinatal Research at Nationwide Childrens's Hospital, and tenured professor in the Department of Pediatrics and Obstetrics/Gynecology at the Ohio State University, College of Medicine, Columbus, Ohio, USA).

Studies: High school in Bucharest, Romania (1941-1944) and Petroşani (1945-1949), then Faculty of Industrial Chemistry at the Bucharest Polytechnic University (1949-1953), followed by three years of stipendiary doctoral studies at the same University under the supervision of Costin D. Nenitzescu (the greatest Roumanian chemist, 1902-1970). The Ph. D. Thesis was entitled "Reactions Catalyzed by Aluminum Chloride", and its results were the basis for two chapters in "Friedel-Crafts and Related Reactions", editor G.A. Olah, Wiley-Interscience, New-York, 1964, "Dehydrogenating Condensations of Aromatics (Scholl and Related Reactions)" by A.T. Balaban and C.D. Nenitzescu, vol. 2. pp. 979-1047, and "Aliphatic Acylation" by C.D. Nenitzescu and A.T. Balaban, vol. 3, pp.1033-1152.

Specialization in Radiochemistry (two semesters 1956-1957) with courses organized by the Bucharest Institute of Atomic Physics.

During all his studies, he was always 1st in his class.

Professional experience (full-time jobs):

1956-1999**,** academic positions at the Chair of Organic Chemistry of the Bucharest Polytechnic University: (assistant professor (1956-1960), associate professor (1961-1966) and full professor (1970-1999) till the mandatory age for retirement.

1967-1974, along with didactic activity, also Head of the Laboratory of Isotopically Labelled Compounds of the Bucharest Institute of Atomic Physics.

1967-1970, Senior Research Officer at the Chemistry Division, International Atomic Energy Agency, Vienna, Austria, in charge with radiopharmaceuticals.

1995-1998, Vicepresident of the Roumanian Academy.

1991-2012, Tenured Professor of Chemistry at the Texas A&M University Galveston, USA TAMUG). It should be emphasized that granting tenure to a 70-year-old European professor is uncommon in USA. Since 2013, after retirement, Professor Emeritus at the same University.

Invited positions (not full-time jobs):

1973, Invited research scientist, Technische Universität Braunschweig, Germany (3 months).

1989-1990, Invited Lectureship, Wilhelm Ostwald Theoretical Organic Chemistry Chair, University Leipzig (6 months).

1991, Invited research scientist, Virginia Commonwealth University, Medical College of Virginia, Department of Medicinal Chemistry, Richmond, Virginia (3 months).

1996, Invited research scientist, Harvard Medical School, Cambridge, MS, US (2 months).

1996, Invited research scientist, École Normale Supérieure, Paris, France (2 months).

Membership in scientific Academies:

1963, elected as corresponding member of the Romanian Academy, Chemistry Section (youngest member among the other 12-14 corresponding members). Only once had a younger person (Nicolae Iorga) been elected in the Roumanian Academy during the previous and later years of the 150-year-old Academy. In 2013 a special issue of *International Journal of Chemical Modeling* was dedicated to the half-century anniversary for this election. Due to political circumstances, the promotion to titular member occurred only after the fall of the communist regime, in 1990.

1983, elected as member of the World Academy of Theoretical Organic Chemists, Paris.

1993, elected as titular member of the Roumanian Academy of Technical Sciences, Bucharest.

1995, elected as titular member of the American-Roumanian Academy of Sciences, Arts and Letters.

2001, elected as honorary member of the Hungarian Academy of Sciences, Budapest.

2005, elected as titular member (and President till 2008) of the International Academy of Mathematical Chemistry, Dubrovnik, Croatia

Honors and Awards:

1962, Roumanian Academy’s Chemistry Prize

1963, Roumanian Order of Labor

1966, Roumanian Order of Scientific Merit

1994, Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society

1997, Doctor Honoris Causa, University of Timişoara Roumania

2000, National Order Star of Romania with grade Faithful Service of the President of Roumania

2007, Roumanian Academy’s Medal “Costin D. Nenitzescu” for distinguished chemical research results

2007, Distinguished Achievement Award for Research of the Association of Former Students, Texas A&M University

2016, National Order Star of Romania with grade Cavalier from the President of Roumania

Scientific Publications:

Books (17**)** among which are mentioned edited [1-4] or authred books [5-11].

It must be emphasized that these books reflect areas where Prof. Balaban has appreciable research results, not covered by any other book.

Chapters in books edited by other authors (over 80).

Articles published in peer-reviewed scientific periodicals (over 800).

Patents (25); three of these are U. S. Patents.

The full list of published books, book chapters, articles and patents has been periodically published in April anniversary issues for 60, 70, 75, 80 amd 85 years oin *Revue Roumaine de Chimie* [12]. Two other journals [13,14] published anniversary issues.

Hirsch index: 62

Membership in Editorial Boards: over 15.

Scientific contributions

Experimental organic chemistry

(selected references cited in a review [13])

Among the results of the Ph. D. thesis are (1) proving that the mechanism of the Scholl reaction (dehydrogenating condensation of aromatic rings) catalyzed Lewis/Brønsted acids [14] involves protonation of one ring followed by electrophilic substitution of the other rings and finally by dehydrogenation or hydride splitting; (2) proving that the $AlCl_3$-catalyzed high-pressure reaction between carbon monoxide and alkanes or cycloalkanes involves as first step the formation of alkyl or cycloalkyl cations which afford acyl cations that subsequently rearrange and/or yield ketones and carboxyl derivatives; (3) more importantly, a new synthesis of pyrylium salts by diacylation of alkenes was discovered. It is now known as a "name reaction": Balaban-Nenitzescu-Praill reaction [15-19]. Independently, it was also reported in 1959 under slightly different conditions in England, and the authors agreed to publish their results back-to-back in the *Journal of the Chemical Society* in 1961 [17]. The pyrylium cation is a benzene ring in which one of the CH groups has been replaced by a positively-charged oxygen atom, and represents therefore the highest single perturbation of an aromatic ring. There is a continuous increase of electron deficiency at one position of the fundamental aromatic unit along the sequence benzene – pyridine – pyridinium – pyrylium. Pyrylium salts are easily formed from acyclic precursors and they undergo ring-opening most easily in the above sequence. Consequently they can serve for synthesizing many acyclic, carbocyclic, or heterocyclic conjugated compounds [20,21]. Prof. A. T. Balaban developed and explored new syntheses based on pyrylium salts during the subsequent decades; he is now considered to be the world authority in this field, being invited to review periodically this field for the *Science of Synthesis* monographs [22,23]. He has written several reviews on pyrylium salts and, with coauthors from Roumania, Germany and Russia, the only existing book in this area [8] . Having the richest collection of pyrylium salts he has investigated systematically all the physical properties of this important class of six-membered aromatic heterocycles (electronic and vibrational absorption spectra, mass spectra, ^{1}H- and ^{13}C-NMR spectra, redox potentials, laser solute activity, charge-transfer spectra with polarizable anions such as iodide, thiocyanate) by collaborating with world-class scientists having the most advanced equipment.

Some products derived from pyrylium salts proved to have practical applications: carbonic anhydrase inhibitors with various biological activities (several publications in collaboration with Claudiu T. Supuran [24], who enriched considerably this field), triaryl-ethylenic anti-tumor reagents, lipophilic pyridinum salts as non-viral gene transfer agents [25], or low-melting point pyrylium and pyridinium salts as ionic liquids.

Another series of papers reported a new synthesis of oxazoles by $AlCl_3$-catalyzed substitution of aromatic compounds with azlactones, followed by dehydration [26].

Distancing himself from Nenitzescu's tradition (they had co-authored 23 papers and 3 book chapters), Prof. Balaban explored new fields, such as new syntheses of indolizines (from pyrylium salts and amino-acetaldehyde ketals) and of naphthalene derivatives (from acetoacetone and benzyl-Grignard reagents).

Isotopic exchange of alkyl hydrogens with deuterium oxide takes place readily for benzylic positions of α or γ alkyl groups of pyrylium cations. The intermediates of such reactions are neutral alkylidene-pyrans, and quantum-chemical calculations explain why α positions are deuterated about ten times faster than γ, whereas the order is reversed for corresponding N-substituted pyridinium salts. With 2,4,6-trimethylpyridine deuterated regioselectively in α or γ or both α and γ it was possible to detect electronic versus steric components of secondary isotope effects, taking into account that CD_3 groups are sterically smaller and more electron-donating than CH_3 groups: protonation depends only on electron density, coordination of bulky metallic complexes depends only on steric effects, and alkylation is affected equally by both types of effects [27].

A simple m ethod for tritiating CH bonds in hydrocarbons and amino acids consists in reacting them with T_2O and $AlCl_3$.

Isotopic labeling of phenathrene with ^{13}C in various positions allowed detecting the degenerate isomerization [28] (for which Prof. Balaban coined the term *automerization*) under catalysis by $AlCl_3$.

The collaboration with physicists in the Bucharest Institute of Atomic Physics who had built their own electronic spin resonance (ESR) spectrometer led to opening a new research area involving persistent nitrogen free radicals. In order to explain the extraordinary stability of hydrazyls such as 2,2-diphenyl-1-picryl-hydrazyl, Prof. Balaban and his co-workers prepared related hydrazyls with lower steric shielding and accordingly lower stability. Then the first push-pull diarylaminyls were synthesized [29] and shown to have stabilities depending both on electronic and steric effects. Then Alan R. Katritzky in England proposed the term merostabilization, whereas Heinz G. Viehe in Belgium came with the term capto-dative stabilization; theoretical analyses had been presented earlier by John W. Linnett and by Michael J. S. Dewar.]

By ESR spectroscopy it was possible to characterize newly synthesized nitroxides [30] and to correlate spin coupling constants with chemical structures. The first N-nitrosoaryl-nitroxides were prepared and shown to be available from NO and nitrosoarenes in reversible reactions. This is a new method for generating the physiologically-active nitric oxide (NO) for which several USA patents were obtained by Prof. Balaban and coworkers in Texas. One of these patents is applied for cosmetic products in China and Taiwan.

Another experimental research direction involves the synthesis of chelate compounds having boron as the central atom. The first such compounds with five-membered chelate rings were prepared from borinic esters and tropolones, and were shown to have high stability and high dipole moments owing to charge delocalization on the tropylium ring. Similar effects occur in analogous borinic compounds with 1,3-dicarbonylic derivatives that have 6-membered chelate rings. Triphenyl-substituted dioxaborinium (boroxaro-pyrylium) cations could be obtained from such systems. The first compounds with 7-membered chelate rings were prepared similarly from dibenzoyl-cyclopentadiene.

Theoretical chemistry

In parallel with experimental chemistry, Professor Balaban had a permanent interest in theoretical chemistry (reviews –[31-34]) starting from simple quantum-chemical calculations for monocyclic aromatic rings (in coll[aboration with his younger colleague Zeno Simon[35]) and continuing with more elaborate calculations involving eminent scientists (Paul v. R. Schleyer, John A. Pople) for the ethane dication which was shown to have a carbonium-carbenium structrure [36]. Dr. Balaban's prediction for the stability of the dioxygen dication with a triple bond was confirmed experimentally.

With two coworkers Dr. Balaban published the first computations on alternative carbon nets, distinct from the honeycomb-like graphite lattice [37]. By analogy with benzenoids, the Balaban and Schleyer system based on the tridimensional of diamondoid hydrocarbons is now generally accepted [38] and has obtained recent attention since rich reserves of diamondoid hydrocarbons were discovered in petroleum. In several collaborations with Professor Douglas J. Klein from TAMUG, other allotropic forms of carbon were discussed, for instance nanocones, nanotubes, and various fullerenes [339,40]. In addition to analyzing nets combining diamond and graphite lattices, Drs. Balaban, Kenneth M. Merz, and Roald Hoffmann published an overview of nets combining symmetrically sp^2- and sp^3-hybridized carbon atoms [41].

Aromaticity occupies a prominent place in Dr. Balaban's interest. Early on, he attempted to enumerate all possible monocyclic aromatic systems starting from the simple reasoning that there are three and only three possibilities for atoms to be part of aromatic rings satisfying Erich Hückel's Rule, namely with 2, 1, or 0 non-hybridized electrons (denoted by X, Y, and Z, respectively) [35]. The corresponding Diophantine equations help in this enumeration, but the topological requirements led to the need for learning graph theory. Not finding in Roumania mathematicians interested in collaborating with him, Professor Balaban contacted Frank Harary, the world specialist in this science. Due to travel restrictions caused by the political situation in Roumania and by the fact that Dr. Balaban's sister and his wife's brother with their families had left the country illegally, Frank Harary had to come to Bucharest and to initiate a collaboration that resulted in 10 joint publications. Many of them solved chemical problems by applying Potya's Theorem. In molecular (constitutional) graphs, vertices symbolize atoms (often hydrogen atoms are not specified), and edges symbolize covalent bonds so that organic chemical formulas may be read as graphs. An essential application for polycyclic aromatic hydrocarbons (benzenoids for short) was using their inner duals (dualists) for classifying them into catafusenes, perifusenes, and coronafusenes according to the nature of their dualists (acyclic, triangle-containing, or larger-ring containing dualists). For catafusenes, a simple code was devised as a unique characterization [41]. With graph-theoretical techniques it was possible to have a global view of all possibilities, and then to select those that had chemical meaning and compatibility (what can be called applying the Sherlock Holmes Principle, *vide infra*). Prof. Balaban published a eries of papers with the general title "Chemical Graphs" [42].

The first book about this interdisciplinary field was edited by Dr. Balaban and appeared in 1976: *Chemical Applications of Graph Theory* [1] and its Chinese translation in 1983. The Foreword to the English Edition was written by Vladimir Prelog. It stressed the possibility of enumerating all isomers for various classes of structures, and emphasized the importance of the adjacency matrix for non-hydrogen atoms, which appears as the Hückel matrix in quantum chemistry.

One area in which cubic (or trivalent) graphs play a dominant role is the enumeration of [*n*]annulene valence isomers $(CH)_n$ where *n* is an even number. With two coauthors, Dr. Balaban published in 1986 on this topic a 3-volume monograph (*Annulenes, Benzo-, Hetero-, Homo-Derivatives and Their Valence Isomers*, [9]. Some of these valence isomers undergo thermal or pohotochemical automerizations. More recently, Dr. Balaban edited in 1997 a book titled *From Chemical Topology to Three-Dimensional Geometry*, , in which various two- and three-dimensional nets were discussed [2].

In the 1940s the first quantitative structure-property relationships (QSPR) were published by Harold Wiener for alkane boiling points at normal pressure, using what would become known as the Wiener topological index. The name "topological index" (TI) would be invented later by Haruo Hosoya for numbers (either integers or real numbers) that are associated with chemical structures in order to assist in predicting quantitatively physical-chemical properties or biological activities (QSAR), important for drug design. Milan Randić, Lemont B. Kier, and Lowell H. Hall developed many successful TIs, using the adjacency matrix of the hydrogen-depleted molecular graph [43]. One of the deficiencies of the TIs that are integers is their high degeneracy (low discriminating ability among isomers), whereas real-number TIs are less degenerate. Another deficiency is the automatic increase of the TI with graph size. On using an approach similar to that imagined by Randić for his connectivity index, but replacing the adjacency matrix by the distance matrix, and compensating graph-size-increase, a new TI was proposed under the name "average distance-based connectivity index *J*", which now is known however as "Balaban index *J*" 44]. Not only is it much less degenerate than all previous TIs, but it allows a simple encoding for the presence of multiple bonds or heteroatoms. Moreover, it is mathematically attractive because for an infinitely long polyethylene chain its value is the number $\pi = 3.14159$ [45]… Many other graph-theoretical chemists have enriched the contributions to molecular descriptors, a few of them in collaboration with Dr. Balaban, including his son, Teodor-Silviu Balaban: Nenad Trinajstić, Ivan Gutman, Subhash C. Basak, Lemont B. Kier, Petru Filip. Other new TIs were studied: several TIs based on informational descriptors, and triplet-based indices that result from converting matrices into systems of linear equations. With one coeditor, Dr. Balaban published a book in 1999 on *topological indices and related molecular descriptors.*

The Lewis acid-catalyzed syntheses of diamondoid hydrocarbons discovered by Schleyer proceed via multiple 1,2-rearrangements. The graph-theoretical analysis of the simplest such reaction involves an ethyl cation with five substituents which undergoes an automerization. This process is characterized by a 20-vertex or a 10-vertex graph depending whether one carbon atom of ethane is or is not labeled. These graphs, published in 1966 [46] constitute the first *reaction graphs*, in which vertices symbolize reaction intermediates and edges symbolize elementary reaction steeps [47]. Interestingly, a few years later the same graphs emerged again, this time representing the pseudorotation of penta-covalent phosphorus compounds.

Graph Theory, Philosophy of Chemistry

Starting from the fact that the 10-vertex graph is known as the 5-cage or the Petersen graph, Dr. Balaban observed relations among the known cages. A few definitions are needed at this stage: when all graph vertices have the same degree (i.e. the same number of edges meet at each point) they are called regular graphs. Cubic or trivalent graphs are regular graphs with degree 3. The girth of a graph is the length of the shortest cycle. The smallest cubic graphs with girth g are called g-cages. In 1970 the known cages had g = 4, 5, 6, 7, 8, and12. Having discovered how a cage with smaller girth *g* was hidden in a cage with girth *g* + 1, Dr. Balaban p[ublished a paper on what was later proved to be the first 10-cage, known as Balaban's 10-cage [48]. Two more 10-cages were found a few years later. In 1973 he found [49] the unique 11-cage, known as Balaban's 11-cage, as was proved by mathematicians using a lengthy computer search. For *g* values higher than 12 there are now only conjectures.

Proposals made by Dr. Balaban about new possibilities for evaluating the performance of researchers, improving the way citations are used for this purpose (e. g. via the Hirsch index) included the use of author indexes of widely-circulated treatises, or modifying the way one considers the impact factors of journals [50]..

Honoring invitations to contribute to special issues of journals dedicated to the philosophy of chemistry, Dr. Balaban published in *Hyle* an essay [51] on how the "Sherlock Holmes principle" (if one eliminates the impossible, then whatever remains, no matter how improbable, must contain the truth) [50] can be implemented by chemical graph theory which allows for instance to find all chemical isomers for a given formula. He commented on Mathematical Chemistry in several journals (*MATCH Communications in Mathematical and Computational Chemistry, Foundations of Chemistry, Fundamenta Informaticae*) [52]. In Pasadena in 2014 he had a keynote lecture titled "What is Mathematical Chemistry?" and published in the *Proceedings of the 38th Annual Congress of the American-Roumanian Academy of Arts and Sciences.*

A Canadian author (Prof. John Andraos) published on the Internet in 2002 "Ph-D-genealogical trees" specifying supervisor names, university locations and years of the doctorate degree. One of the Liebig genealogical trees follows.

Justus von Liebig 1803-1873 (Erlangen, 1822) →

Heinrich Will 1812-1890 (Giessen, 1839) →

August Kekule 1829-1891 (Giessen, 1852) →

Theodor Zincke 1843-1928 (Goettingen, 1869) →

Hans Fischer 1881-1945 (Marburg 1904; Chemistry Nobel Prize 1930) →

Costin D. Nenitzescu 1902-1970 (TH Munich , 1925; Nenitzescu synthesis of indoles 19229; Nenitzescu reductive acylation) →

Alexandru T. Balaban 1931- (TH Bukarest1959; Balaban- Nenitzescu-Praill synthesis of pyrylium salts).

Bibliography

Edited or co-edited books:

1. A.T. Balaban (editor): "Chemical Applications of Graph Theory" Academic Press, London, 1976,. Chineese translation, 1983.
2. A.T. Balaban (editor), "From Chemical Topology to Three-Dimensional Geometry", Plenum Publishing Corporation, New York,1997
3. A.T. Balaban, E. N. Carabateas, and F. A. Tanasescu (editors),, "Science and Technology Management", NATO Science Series (Series 4: Science and Technology Policy, Vol. 22), Proc. of NATO Advanced Research Workshop (Sinaia, Romania, May 20-24, 1997) IOS Press, Series 4, vol. 22, Amsterdam, 1998
4. J. Devillers and A.T. Balaban (editors), "Topological Indices and Related Descriptors in QSAR and QSPR" Gordon and Breach, The Netherlands, 1999. 811 pages.

Aithored or c-authored books:

5. A.T. Balaban, A. Chiriac, I. Motoc and Z. Simon, "Steric Fit in Quantitative Structure Activity Relations", Lecture Notes in Chemistry No. 15, Springer Verlag, Berlin, 1980, 178 pages.

6 V. Dragutan, A.T. Balaban and M. Dimonie, "Olefin Metathesis and Ring-Opening Polymerization of Cyclo-Olefins", Editura Academiei Romane, Bucharest, 1981, 254 pages (in Roumanian); Expanded English version: Wiley, Chichester, 1985, 545 pages.

7. A.T. Balaban, I. Galateanu, G. Georgescu and L. Simionescu, "Labelled Compounds and Radio-pharmaceuticals Applied in Nuclear Medicine", Editura Academiei Romane, Bucharest, 1979, 495 pages (in Roumanian); Expanded English version: Wiley, Chichester, 1988, 742 pages.
8. A.T. Balaban, A. Dinculescu, G.N. Dorofeenko, G.W. Fischer, A.V. Koblik, V.V. Mezheritskii and W. Schroth, "Pyrylium Salts. Syntheses, Reactions and Physical Properties", Advances in Heterocyclic Chemistry, Suppl. Vol. 2 (A. R. Katritzky, Ed.), Academic Press, New York, 1982.
9. A.T. Balaban, M. Banciu and V. Ciorba, " Annulenes, Benzo-, Hetero-, Homo-Derivatives and Their Valence Isomers", CRC Press, Boca Raton, Florida, 1986, 3 volumes.

10. N. Voiculetz, A.T. Balaban, I. Niculescu-Duvaz and Z. Simon, Modeling of Cancer Genesis and Prevention", CRC Press, Boca Raton, Florida, 1990.

11. M. Banciu and A.T. Balaban, "C.D. Nenitzescu: His Life and His Work" (in Roumanian), Editura Academiei Romane, Bucharest, 1995.

Anniversary issues of sciemntific periodicals

12. *Revue Roumaine de Chimie* 1991, **26**, 289-301; 2001, **46,** 265-275; 2006, **51,** 240-244; 2011, **56**, 279-288; 2016, **61**, 243-246 (list of sciemtific publications in the preceding 10 or 5 years).

13. *Archives for Organic Chemistry (ARKIVOC)* 2006 (x) 1-352.

14. *MATCH, Communications in Mathematical and Computer Chemistry*, 2011. **66**, 1-32: Autobiographical notes: 80 years of age, 68 years of chemistry; Romanian translation, *Buletinul Soc. Chim. Romania* 2011, 18 (2) 21-46.

Book chapters and articles in scientific periodicals

13. A. T. Balaban, *Rev. Roum. Chim.* 2012, **57**, 535-557: Brief review of contributions to organic chemistry.

14. A. T. Balaban and C.D. Nenitzescu: "Dehydrogenating Condensations of Aromatics (Scholl and Related Reactions)", in "*Friedel-Crafts and Related Reactions",* editor G.A. Olah, Wiley-Interscience, New-York, 1964, vol. 2. pp. 979-1047.

15. C. D. Nenitzescu and A.T. Balaban: "Aliphatic Acylation", in "*Friedel-Crafts and Related Reactions*", editor G.A. Olah, Wiley-Interscience, New-York, 1964,, vol. 3, pp.1033-1152.

16. A.T. Balaban and C.D. Nenitzescu, *Liebigs Ann. Chem*., 1959, **625**, 74-88: Reactions catalyzed by aluminium chloride. XXVII. A synthesis of pyrylium salts from acid chlorides and olefins (in German).

17. A.T. Balaban and C.D. Nenitzescu, *J. Chem. Soc.*, **1961**, 3553-3560: Pyrylium salts obtained by diacylation of olefins. II. The two pyrylium salts formed in the diacylation of 2-methyl-2-butene; P. F. G. Praill and A. L. Whitear, *J. Chem. Soc.* **1961**, 3573: Pyrylium salts and related compounds. Part I. The reaction between olefins and acylium perchlorates.

18. A. Hassner and C. Stumer, *Organic Syntheses Based on Name Reactions*, 2nd Ed., Elsevier, Amsterdam, 2002, p. 17.

19. A. T. Balaban, Balaban-Nenitzescu-Praill Reaction, In: *Name Reactions in Heterocyclic Chemistry II* (J. J. Li, ed.) with a foreword by E. J. Corey. Wiley, Hoboken, NJ, 2011, pp. 402-419.9

20. A.T. Balaban, “Pyrylium salts as useful synthons”, in “*Organic Synthesis : Modern Trends*” (ed. O. Chizov), Blackwell, Oxford, 1987, pp. 263-274.
21. A.T. Balaban, W. Schroth and G. Fischer, “Pyrylium Salts. I. Synthesis”, in *Advances in Heterocyclic Chemistry*, (eds. A. R. Katritzky and A. J. Boulton), Academic Press, New York, 1969, vol. 10, pp. 241-326.
22. W. Schroth and A.T. Balaban, “Pyrylium-Salts” in *Methoden der Organischen Chemie (Houben-Weyl*)”, vol. E7b, Hetarene II (Teil 2), (R.P. Kreher, Ed.), G. Thieme Verlag, Stuttgart, 1992: Introduction (pp. 755-766); Synthesis (pp. 767-963) (in German).
23. T.S. Balaban and A.T. Balaban, “Pyrylium Salts”. In “*Science of Synthesis; Houben-Weyl Methods of Molecular Transformations*”, Georg Thieme Verlag, Stuttgart, 2003, vol. 14, pp. 11-200; A. T. Balaban and T. S. Balaban, in : *Science of Synthesis, Knowledge Updates 2013/3:* Pyrylium Salts (Update 2013)m Thieme Verlag, 2013, Stutttgart, pp. 145-216.
24. Ö. Güzel, A. Maresca, A. Scozzafava, A. Salman, A. T. Balaban, and C. T. Supuran, J. Med. Chem. 2009, **52**, 4063-4067: Discovery of nanomolar and subnanomolar inhibitors of the mycobacterial β carbonic anhydrases Rv1284 and Rv3273.
25. M. A. Ilies, W. A. Seitz, M. T. Caproiu, M. Wentz, R. E. Garfield, and A. T. Balaban, *Eur. J. Org. Chem.* **2003**, 2645-2655: Pyridinium-based cationic lipids as gene transfer agents.
26. A.T. Balaban, L. Birladeanu, I. Bally, P.T. Frangopol, M. Mocanu, and Z. Simon, *Tetrahedron*, 1963, **19**, 2199-2207: Preparation and spectra of *para*-substituted 2,5-diphenyloxazoles (Aminoketone synthesis. VI).
27. A. T. Balaban, “Steric versus electronic effects of deuterium”, in “*Synthesis and Applications Isotopically Labelled Compounds*” (eds. W.P. Duncan and A.B. Susan), Pr. F. Liebman andA. Greer)., Chapter X, Wiley, 2018, pp. 1–9.
30. A9.T. Balaban, E.U. Würthwein and P. von R. Schleyer, *Tetrahedron*, 1987, **43**, 405-408: Model MNDO calculations for rotamers of α-acylnitroxides and of N-nitrosonitroxides.
31. .T. Balaban, I. Bally, R.J. Bishop, C.N. Rentea and L.E. Sutton, *J. Chem. Soc*. **1964**, 2382-2387: Novel spiroborates and a dipole moment study of 1,3,2-dioxabora-azulene-2-spiro-2’-(1’,3’,2’-benzodioxaborole).(Heterocyclic organoboron compounds. II.).
32. A. T. Balaban, Confessions and reflections of a graph-theoretical chemist; *MATCH, Commun. Math. Comput. Chem.* 1993, **29,** 3-17.

33. A. T. Balaban, *Internet Electronic J. Mol. Design* 2012, **11**, 1-22.C A personal view of chemistry (with emphasis to mathematical chemistry) as science and art.
34. A. T. Balaban, *J. Chem. Inf. Comput. Sci*. 1995, **35**, 339-350: Chemical graphs: looking back and a glimpse ahead,
35. A.T. Balaban and Z. Simon, *Tetrahedron*, 1962, **18**, 315-321: Aromaticity constants.
36. P. von R. Schleyer, A.J. Kos, J.A. Pople and A.T. Balaban, *J. Amer. Chem. Soc.*, 1982, **104**, 3771-3773: Carbenium-carbonium structure H_2C^+-CH_4^+, for the ethane dication.
37. A.T. Balaban, C.C. Rentea and E. Ciupitu, *Rev. Roum. Chim.*, 1968, **13**, 231-247: Chemical graphs. VI. Estimation of the relative stability of several planar and tridimensional lattices for elementary carbon (Erratum, *ibid.*, p. 1233).
38. A.T. Balaban and P. von R. Schleyer, *Tetrahedron,* 1978, **34**, 3599-3609: Systematic classification and nomenclature of diamond hydrocarbons. 1. Graph-teoretical enumeration of polymantanes.
39. A.T. Balaban, D.J. Klein and C.A. Folden, *Chem. Phys. Lett.* 1994, **217**, 266-270: Diamond-graphite hybrids.
40. A. T. Balaban and D. J. Klein, *J. Phys. Chem. C*, 2009, **113**, 19123-19133: Claromatic carbon nano-structures.
41. K.M. Merz Jr., R. Hoffmann and A.T. Balaban, *J. Amer. Chem. Soc.*, 1987, **109**, 6742-6751: 3,4-Connected carbon nets : through-space and through-bond interactions in the solid state.
41. A.T. Balaban and F. Harary, *Tetrahedron,* 1968, **24**, 2505-2516: Chemical graphs. V. Enumeration and proposed nomenclature of benzenoid *cata*-condensed polycyclic aromatic
42. C. Deleanu and A.T. Balaban, *Rev. Roum. Chim.*, 1990, **35**, 349-391: Chemical graphs. Part. 53. Benzo- and polybenzo-derivatives of valence isomers of [12]annulene.
43. A.T. Balaban, L.B. Kier and N. Joshi, *J. Chem. Inf. Comput. Sci.*, 1992, **32**, 237-244: Correlation between chemical structure and normal boiling points of acyclic ethers, peroxides, acetals,and their sulfur analogues.
44. 42. A.T. Balaban, *Chem. Phys. Lett.*, 1982, **80**, 399-404: Highly discriminating distance-based topological index.
45. A.T. Balaban, N. Ionescu-Pallas and T.S. Balaban, *MATCH*, Commun. *Math.Compit. Chem.* 1985, **17**, 121-146: Asymptotic values of topological indices *J* and *J'* (average distance sum connectivities) for infinite acyclic and cyclic graphs.

46. A.T. Balaban, D. Farcasiu and R. Banica, *Rev. Roum. Chim.*, 1966, **11**, 1205-1227: Chemical graphs. II. Graphs of multiple 1,2-shifts in carbonium ions and related systems.

477. A.T. Balaban, “Reaction graphs”, in “*Graph Theoretical Approaches to Chemical Reactivity*”, (eds. D. Bonchev and O. Mekenyan), Kluwer Academic Publishers, Dordrecht,8Netherlands, 1994, pp.137-180.

48. A.T. Balaban, *J. Combinatorial Theory, Ser. B*, 1972, **12**, 1-5: A trivalent graph of girth ten.

49. A.T. Balaban, *Rev. Roum. Math. Pures Appl.,* 1973, **18**, 1033-1043: Trivalent graphs of girth nine and eleven, and relationships among cages.

50. A.T. Balaban, *Scientometrics,* 1996, **37**, 495-498: How should citations to articles in high- and low-impact journals be evaluated, or what is a citation worth ?

51. A. T. Balaban, *Hyle* 2013, **19**, 106-134: Chemical graph theory and the Sherlock Holmes principle,

52. A. T. Balaban, *Foundations Chem.* 2005, **7**, 289-306: Reflections about mathematical chemistry.