communications in mathematical
match
and in computer chemistry

no. 44, October 2001

MATCDY (44) 5 - 13 (2001)

ISSN 0340 - 6253

ALEXANDRU T. BALABAN – CHEMISTRY BETWEEN LABORATORY AND COMPUTER

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This special issue of MATCH is dedicated to the occasion of the 70th birthday of Professor Alexandru T. Balaban, one of the few of today's chemists who continues the Renaissance ideal of a complete scientist, with original accomplishments both in organic, bio-organic, and theoretical chemistry, and in computer-assisted drug design.

Professor Alexandru T. Balaban (Sandy) studied organic chemistry and received a Ph.D. in organic chemistry at the Polytechnic University, Bucharest, Romania, followed by a D. Sci. in 1972. Between 1956 and 1999 he held a Professorship at the same University, teaching organic chemistry and general chemistry. Between 1961 and 1975 he was also head of the Laboratory for Isotopically Labeled Compounds from the Institute of Atomic Physics (Bucharest, Romania), and between 1967 and 1970 he was senior research officer at the International Atomic Energy Agency (Vienna, Austria). In 1963 he was elected as corresponding member and from 1990 titular member of the Romanian Academy, whose vice-president he was between 1995 and 1998. In 2001 he was elected as honorary member of the Hungarian Academy of Sciences. He is now professor of organic chemistry at the Texas A&M University at Galveston, Texas, where he continues his research both in experimental and theoretical chemistry. Author of over 600 papers, and more than 50 chapters in books, nine authored books and seven edited books, he was visiting professor in the U.S.A., France, and Germany, and in 1994 he received the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society. Recognized as a scientific leader in various branches of chemistry, he serves on the editorial boards of Revue Roumaine de Chimie and Revista de Chimie (Bucharest), and of several international journals: Fullerene Science and Technology, Polycyclic Aromatic Compounds, Organic Preparations and Procedures International, MATCH, SAR and QSAR in Environmental

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Research, Journal of Radioanalytical and Nuclear Chemistry, Heterocyclic Communications, Advances in Heterocyclic Chemistry, and Scientometrics. He also was a member of the editorial boards of Journal of Chemical Information and Computer Sciences, Journal of Labeled Compounds and Radiopharmaceuticals, Journal of Computational Chemistry, and Journal of Mathematical Chemistry.

Starting with research in the chemistry of pyrylium salts, he touched many important subjects of organic and bio-organic chemistry: homogeneous catalysis under acid conditions (he investigated reactions catalyzed by Lewis and Brønsted acids); heterocyclic compounds (he discovered new syntheses of pyrylium salts by olefin diacylation, and wrote the first book and several book chapters on pyrylium salts; he is co-author of a new synthesis of oxazoles and thiazoles); stable free radicals (he prepared the first aminyls stabilized by push-pull electronic effects, and the first N-nitroso-nitroxides); catalytic isomerizations of polycyclic aromatic hydrocarbons (he introduced the term automerization, and demonstrated the catalytic automerization of phenanthrene labeled with carbon-13 under the influence of aluminum chloride); isotopically labeled compounds (he proposed new syntheses for labeling organic molecules with deuterium, tritium, and carbon-14); nitric oxide donors (he developed new NO donors, solutions of NO in fluorocarbon emulsions, and NO-developing gels); ionic liquids and cationic lipids (in both cases the products are pyridinium salts prepared *via* pyrylium salts).

Because this *Journal* and the papers from this special issue treat subjects from mathematical and theoretical chemistry, we will present more details regarding the activity of Professor Balaban in this field. He edited the first book on chemical applications of graph theory [1], being one of the early developers and proponents of the field of chemical, particularly molecular, graphs. The interplay between chemical topology and the three-dimensional structure of chemical compounds was the subject of a recent book [2]. In several highly appreciated and cited reviews he presented to the chemical community the directions where chemical graphs can be successfully applied [3-8]. At a time when the characteristic polynomial was thought to be a complete graph invariant, he and Harary demonstrated that this is not true [9]. Other chemical graph papers were dedicated to trivalent graphs [10,11] and computer generation of all cycles in a graph [12].

The enumeration of isomers [13] is another topic where he made important contributions [14-21], mainly for alkanes and different classes of benzenoid hydrocarbons. Connected with his interest in benzenoid hydrocarbons is the enumeration of Kekulé structures [22-24]. A very efficient coding algorithm, the hierarchically ordered extended connectivities procedure, was developed together with Mekenyan and Bonchev [25]. His interest in organic chemistry was the inspiration for the introduction of reaction graphs [26], which found applications for the 1,2-shifts in carbonium ions [27], six-membered transition states [28], rearrangements of tetragonal-pyramidal complexes [29], rearrangements of XeF_6 [30], or rearrangements of pentagonal-bipyramidal complexes [31].

The first book on the valence isomers of annulenes, and their benzo-, hetero-, and homo-derivatives was published together with Banciu and Ciorba [32]. He was the first to publish an exhaustive listing and the interconversions of valence isomers for various classes of compounds [33-37], mainly for $(CH)_{2k}$ hydrocarbons.

He was an advocate for the use of topological indices in QSPR and QSAR studies, and he introduced many new molecular matrices, graph invariants, and topological indices

[38-42]. The first book dedicated entirely to topological indices was edited by him together with Devillers [40]. The most important topological indices proposed by Balaban are mentioned here: *J*, a highly used index in QSPR, QSAR, and for the virtual screening of combinatorial libraries [43,44]; the triplet indices **T.P.R** [45]; regressive vertex degree and vertex sum indices, developed with Diudea [46,47]; the information-theory indices *U*, *V*, *X*, and *Y* [48,49]. Many topological indices are derived from molecular matrices, and he proposed the maximum path (detour) matrix [50], reciprocal distance matrix [51], complementary distance matrix [52], and reverse Wiener matrix [53]. He also introduced several weighting schemes for computing atom and bond parameters in molecular graphs containing heteroatoms and multiple bonds [54-56].

He is an active promoter for the use of topological indices in QSAR and QSPR studies [57-59] and his papers present significant success stories in this very active domain: octane numbers for hydrocarbons [60,61], boiling point temperature [62-65], anticancer activity [66-68].

The study of allotropic forms of carbon [69,70] started in 1968 when he published the first paper on possible alternative carbon nets, different from diamond or graphite [71]. These studies were continued in joint papers with Hoffmann [72] about 3,4-connected carbon nets and Klein [73,74] about diamond-graphite hybrids and graphitic cones; he predicted the existence of graphitic cones before they were observed. He continued recently with several interesting theoretical investigations of fullerene-like compounds, hetero-nanotubes, pillow fullerenes, and other cage compounds [75-83]. He also published several papers about graph-theoretical invariants for fullerenes [84-86].

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