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PREFACE

Preface

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This issue is devoted to the anniversary meeting "*20 Years of Molecular Topology in Cluj*", TOPMOL 2006, held in Cluj-Napoca, Romania, Europe, in the period September 25–30, 2006. The conference which joined 45 of the leading researchers in the field of Graph Theory, QSAR/QSPR and Nanoscience, from Europe, America and Asia, was developed under the honorary auspices of Romanian Society of Chemistry and the International Academy of Mathematical Chemistry.

In the year 1986, the TOPO GROUP CLUJ (at the Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University, Cluj, Romania) was established and since then a multitude of work, participation at national and international scientific manifestations, several finished PhDs, several Romanian grants, articles and books, as well as software have been associated with our group.

Collaboration with our European neighbors has priority, so that the TOPO GROUP CLUJ has manifested interest in integration of the research directed at the main common themes, such as drug design, nanoscience or molecular topology, establishing contacts based on our own original results, first towards the former Yugoslavian countries, followed by Germany and UK. In twenty years of activity (1986–2007), the TOPO GROUP CLUJ has published scientific articles in collaboration with scientists of 16 countries: 1. Bulgaria (1); 2. China (1); 3. **Croatia (20)**; 4. Cuba (2); 5. **Germany (18)**; 6. Hungary (4); 7. India (3); 8. Iran (1); 9. Israel (1); 10. Japan (2); 11. Macedonia (3); 12. Russia (2); 13. **Serbia (7)**; 14. **Slovenia (5)**; 15. UK (4) and 16. SUA (3).

Other collaborations have developed in connection with several edited books: M. V. Diudea, (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, **NOVA**, New York, 2001; M. V. Diudea; O. Ivanciuc, (Eds.), *MATCH Commun. Math Comput.*

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Chem., 2001. M. V. Diudea, (Ed.), *Nanostructures—Novel Architecture*, **NOVA**, New York, 2005, in collaboration with the following countries:

1. Belgium (1); 2. **Croatia (4)**; 3. **Germany (3)**; 4. Hungary (4); 5. Japan (2); 6. Macedonia (1); 7. Russia (2); 8. Serbia (1); 9. Slovenia (1); 10. Spain (2); 11. UK (2); 12. **USA (6)** and 13. Taiwan (1).

Among **180 published** articles, a total of **60 articles** with international collaboration (of which **44** are **ISI** quoted), furthermore **65 ISI** quoted papers (without collaboration), and **12 books** (including edited books and journal issues—of which 4 were published in Romania), and 8 original software programs form the main output of the TOPO GROUP CLUJ.

In addition to these results, one should mention the *reviewing* activity at several prestigious journals (1. *Rev. Roum. Chim*.; 2. *Studia Univ. Babes-Bolyai*; 3. *Croat. Chem. Acta*; 4. *J. Chem. Inf. Comput. Sci.*; 5. *Chem. Phys. Lett.*; 6. *Int. Elect. J. Mol. Design*; 7. *New J. Chem*.; 8. *SAR/QSAR Env. Res*.; 9. *Bioorg. Med. Chem. Lett.*; 10. *MATCH*, *Commun. Math. Comput. Chem*.; 11. *Fullerenes, Nanotubes Carbon Nanostruct.*; 12. Molecules; 13. *J. Am. Chem. Soc.*; 14. *Romanian Chem. Quart. Revs*; 15. *Ars Combinatorica*; 16. *Arkivoc*; 17. *Utilitas Math.*; 18. *Eur. J. Operational Res.*; 19. *Math. Comput. Model.*; 20. *J. Org. Chem*.) and the activity in advisory boards of some journals in the field (1. *Croatica Chemica Acta*, 1996-; 2. *Studia Univ*. "*Babes-Bolyai*", 1999–2005; 3. *Acta Univ. Cibiniensis*, 1999-; 4. *MATCH,Commun. Math. Comput. Chem*., 2000-; 5. *Internet Electronic Journal of Molecular Design* 2001-; 6. *Carpathian J. Math., 2005*-; 7. *Current Drug Discovery Technologies*, 2007).

In 2007 the TOPO GROUP CLUJ has founded the European Society of Mathematical Chemistry, which was registered at the Court of Cluj, Romania. Founding members of this society are important scientific personalities from Romania, Europe but also from America and Asia, certifying the role played by Romania in the scientific realm of Europe and the World.

In the present issue, the main scientific directions represented are presented below.

QSAR

QSAR models based on two different similarity methods were developed to predict two enzyme kinetic parameters for catecholic substrates of human soluble catechol *O*-methyl-transferase (A. Costescu, C. D. Moldovan, G. Katona and M. V. Diudea), and the Log P of a set of 38 of 2-furylethylenes was modeled by using topological indices (C. D. Moldovan, A. Costescu, G. Katona and M. V. Diudea).

Graph theory

The definition of the path-Zagreb matrix for (chemical) trees *PZ* and its generalization to any (molecular) graph is presented (D. Vukičević, S. Nikolić and N. Trinajstić).

Optimal configurations of functionalized fullerenes $C_{60}X_n$ for $n = 2, 4, 6, 8$ have been determined by application of three topological stability measures (D. Vukičević and A. Graovac).

Subgraphs obtained by applying several fragmentation criteria are investigated, also the matrix and polynomial representations of vertices composing each type of subgraphs were given (L. Jäntschi and M. V. Diudea).

An alternative method for solving homogenous and non-homogenous linear differential equation systems used in chemical kinetics and pharmacokinetics on the basis of flow graph principles is proposed (M. Socol and I. Bâldea).

It has been shown that the boundary structure of patches with all faces of the same size k, all interior vertices of the same degree m and all boundary vertices of degree at most m determines the number of faces of the patch (G. Brinkmann, J. E. Graver and C. Justus).

Software and computation

A novel software framework (GrInvIn–Graph Invariant Investigator) for teaching graph theory and for research in graph theory and graph theoretic chemistry is presented in a nutshell (A. Peeters, K. Coolsaet, G. Brinkmann, N. Van Cleemput and V. Fack).

The software to generate Zagreb matrices and related descriptors for (molecular) graphs (D. Vukičević and S. Nikolić).

An optimized algorithm for finding all symmetry-distinct maps of a given graph is described (E. Lijnen and A. Ceulemans).

A method for scheduling collective communication routines that are used in parallel MD and are based on the property that the graphs in question have a Hamilton cycle (K. Kutnar, U. Boršnik, D. Marušič and D. Janežič).

Communication algorithms, tailored for molecular dynamics simulation on d-meshes, are evaluated in terms of communication efficiency (R. Trobec, U. Borštnik, and D. Janežič).

Kekulé structure counting

Analytical formulas for calculating the Kekulé structure number for families of polyhex tori are derived by using the transfer matrix method (D. Vukičević, S. Cigher and M. V. Diudea).

Generation of all geometric Kekulé structures for families of polyhex tori of a given tube cross-section, was performed by the new Kekulé Count software, developed on a coloring algorithm (S. Cigher, D. Vukičević and M. V. Diudea).

On The Kekulé Number Of Leapfrog Fullerenes (K. Kutnar, D. Marušič and D. Vukičević) and On the Anti-Kekulé Number of Leapfrog Fullerenes (K. Kutnar, J. Sedlar and D. Vukičević).

Polynomials

A novel class of counting polynomials, called Cluj polynomials is proposed on the ground of Cluj matrices and the Utility of Cluj descriptors in predicting the resonance energy of a set of planar polyhexes is exemplified (M. V. Diudea).

The newly proposed Omega counting polynomial is investigated in case of twisted/chiral polyhex tori (M. V. Diudea).

Use of Omega polynomial in the description of small fullerenes and tubular nanostructures (M. V. Diudea, S. Cigher, A. E. Vizitiu, M. S. Florescu and P. E. John).

Analytical expressions for Hosoya polynomials of TUC4C8(S) nanotubes (S. Xu and H. Zhang).

Nano science

The aromaticity of a novel class of non-classical fullerenes, having pentagon-heptagon pairs as in azulene, is discussed in the light of several criteria (M. V. Diudea and A. E. Vizitiu).

Retro-leapfrog operation used for structure elucidation (M. V. Diudea).

It is shown that the through-bond currents in a closed molecular network originate from their topologically invariant edge-homologies (E. Lijnen, A. Ceulemans, M. V. Diudea and Cs. L. Nagy).

The structure and stability of axially elongated carbon tori obtained by connecting the adjacent walls of an armchair DWCNT is studied (Cs. L. Nagy, K. Nagy and M. V. Diudea).

Tight-binding energy-band calculations for a series of proposed carbon nanostructures in the shape of tetrapod as three-dimensional junctions for carbon nanotubes shows that their electronic property depends on one topological factor (K. Nakada, K. Maeda and K. Daigoku).

New tubercular fulleroids have been built up by using the three classical composite map operations: tripling (leapfrog *Le*), quadrupling (chamfering *Q*) and septupling (capra *Ca*) on the trivalent Platonic solids (A. E. Vizitiu, Cs. L. Nagy, M. Stefu, G. Katona, M. V. Diudea, B. Parv and D. Vukičević).

In addition, two contributions from the broader fields of mathematical chemistry are presented (P. G. Mezey).

This issue is aimed to be a bridge between basic and applied theory, with strong connections to the educational field. The guest Editor is grateful to all of the contributors for their efforts to produce good quality articles, which help to the promotion of Mathematical Chemistry and also the European Society of Mathematical Chemistry. Acknowledgements are expressed to Prof. Paul Mezey, the Editor in Chief of Journal of Mathematical Chemistry, for the opportunity in publication of this issue.

Cluj, August 4, 2008 Prof. Dr. Mircea V. Diudea.