Ante Graovac and Chemical Graph Theory

Ante Graovac (Split, Croatia, July 15, 1945 – Zagreb, Croatia, November 13, 2012), a theoretical physicist, was a member of the Advisory Board of our journal from its inception in 2008. In 2014, a book about his life and work was published in Kragujevac, Serbia [2]. His technical work speaks for itself. We can only add that Ante was a larger than life character, known amongst mathematical chemists for his enthusiasm, kindness, and readiness to collaborate. He had a real talent for bringing colleagues together, formally and informally.

Ante Graovac also has a special place in field of this journal. Only now that we look back, can we see how significant was his role in the development of mathematical chemistry/chemical graph theory in Slovenia, his native Croatia, other countries of former Yugoslavia and beyond. Together with mathematician Dragoš Cvetković, chemists Ivan Gutman, Nenad Trinajstić and physicist Milan Randić he was a pioneer in the field of chemical graph theory, mainly in connection with applications of linear algebra to chemically motivated problems. One of the earliest systematic treatments of this graph-theoretical or 'topological' approach to conjugated molecules was a volume in the Springer Lecture Notes Series co-authored by Graovac, Gutman and Trinajstić [1]. In the seventies and early eighties, his favourite graphs were benzenoids and other planar molecular graphs arising from hydrocarbons. Later, like many in the field who were inspired by the revolution in carbon chemistry and physics that led to the award of the fullerene and graphene Nobel prizes, respectively, to Curl, Kroto and Smalley (Chemistry, 1996) and to Geim and Novoselov (Physics, 2010), Ante turned to exploration of features of many other types of carbon framework.

In particular, in the eighties, after the discovery of buckminsterfullerene by Kroto, Smalley and Rice, he became fascinated with fullerenes. It was Ante who brought the late Harry Kroto by train from Zagreb to Ljubljana, a few months before Harry shared the Nobel Prize. In the nineties, Ante worked with us and others on the remarkable property of some graphs that they 'know' how to draw themselves. In addition to our many pairwise interactions, the three of us (AG, TP and PWF) have a single paper in common. This deals with a generalisation of the face-spiral approach for description and enumeration of cubic polyhedra, especially fullerenes.

In 1985 W. Imrich, the late T. D. Parsons (thesis advisor of TP) and TP organised an international conference in Dubrovnik at which Ante also took part. The success of the conference motivated Ante to start, a year later, a series of unusual, but very successful annual summer schools, workshops and conferences Math/Chem/Comp which charted the territory of chemical graph theory.

Ante was among the founding members of the International Academy of Mathematical Chemistry. He served as its secretary until his untimely death. Although he spent most of his working life at the Ruđer Bošković Institute in Zagreb and the University of Split, his work in Mathematical Chemistry inspired many younger colleagues at home and abroad to take up this interdisciplinary subject. Let us mention just Damir Vukičević and Tomislav Došlić. Throughout his life Ante maintained a strong friendship with Ivan Gutman. Ivan, with his editorship of the journal MATCH, and Ante with his Math/Chem/Comp meetings were important sources of inspiration for mathematicians starting up this field in several countries.

Algebraic and Topological Graph Theory, IUC, Dubrovnik, 1985, organised by Imrich, Parsons and Pisanski. Ante Graovac with glasses in the last row. The meeting was an inspiration for Ante's Math/Chem/Comp meetings. (Photo: Vladimir Batagelj)

Although mathematical chemistry is a prime application of combinatorics, and dates back to the 19th century with the first treatments of enumeration problems of alkanes, it received important new impetus from Hückel theory in the early 20th century with the explicit connection of quantum mechanics to linear algebra. Kekulé structures alias perfect matchings continue to inspire applications of graph theory. Numerous graph invariants, also known as topological indices of molecular graphs have been devised to represent, with varying degrees of success, physical and chemical properties of molecules from calculable properties of the molecular graph. In the last decade, graph theory in chemistry has received another fillip, from its new-found applicability to the theory of molecular conduction, another field represented in this volume.

It seems fair to say that mathematical chemistry of the mid-twentieth century was a subject practiced mostly by theoretical chemists and was looked upon with a certain scepticism by mathematicians. One aim in editing this volume was to show that discrete mathematical chemistry does offer questions worthy of serious mathematical study and can benefit from the contributions of mathematical professionals. The present volume of AMC consists of 15 papers from this field, many written by mathematicians alone or in collaboration.

Patrick Fowler and Tomaž Pisanski
Guest Editors

References

[1] A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, volume 4 of *Lecture Notes in Chemistry*, Springer-Verlag, Berlin, 1977, 123 pages.

[2] I. Gutman, B. Pokrić and D. Vukičević (Eds.), *Ante Graovac – Life and Works*, volume 16 of *Mathematical Chemistry Monographs*, University of Kragujevac, Kragujevac, 2014, 306 pages.