Sixth International Conference on Mathematical Chemistry

Organizers: E. C. Kirby and D. H. Rouvray

Special themes: The role of fuzzy logic in chemistry
The role and definition of chemical concepts

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Scientific meetings often have quite a long gestation period, and this one was no exception. It was conceived several years ago when the two organizers, who had independently been thinking along similar lines, came together. They wanted to arrange a meeting that was a little out of the ordinary, and one where participants could re-examine a number of concepts that are fundamental in chemistry. Participants would be encouraged to step back a little from the workbench, desk, or computer and ask questions about what they were thinking and where chemistry was going. Questions such as how useful are the concepts that are currently accepted? How well-founded are they? We have all heard those entertaining myths of science that tell of the sudden arrival of brand new ideas or sharp pictorial images (Archimedes, Kekulé, and so on). In reality, most concepts seem to start life as rather vague mental constructs. Typically it is only after a great deal of hard work that they can be pinned down with sufficient formality and precision to become presentable to the scientific community at large. Ideally, a concept thus launched will, if it is accepted, be subjected to increasingly rigorous examination as knowledge of it spreads. But an interesting question needs to be asked at this point. *Can* chemical concepts always be defined precisely and rigorously, or is it possible that, at least sometimes, inspirational and explanatory power may be lost in the endeavor to formalize them, thus denying their inherently intuitive, arbitrary, and sometimes paradoxical nature? The real physical world is often a far more messy and complex place than many of our simplistic ideas allow for. Was the Dutch physicist H. A. Kramers in fact right when he declared that "in the world of human thought generally and in physical science in particular, the most important and fruitful concepts are those to which it is impossible to attach a well-defined meaning"? At this point it seemed only natural to include a serious look at whether the fast developing field of fuzzy logic might also have a part to play in the conference proceedings. The organizers felt that it did and that a whole day should be allocated to this topic.

This, in summary, was how the overall theme of the conference was conceived and developed. Subsequently the International Society for Mathematical Chemistry, while gathered in Kansas City in May 1993 for its Fifth International Conference, adopted these ideas and gave its endorsement to the organizers as they proceeded with arrangements for what was to become the Sixth International Conference.

The international meetings in this current series were started by Professor Bruce King of the University of Georgia, and the first of these held at the University of Georgia, Athens, Georgia in April 1983. The second meeting of the series was also held at the University of Georgia, in 1987, this time organized jointly by Professor King and Dr. Dennis Rouvray. It was at this meeting that the Journal of Mathematical Chemistry edited by Dennis Rouvray was launched and that the International Society of Mathematical Chemistry became established. Subsequent meetings were held in 1989 at Galveston, TX; in 1991 at Bled, then in Yugoslavia, but now in Slovenia; and, as mentioned, in 1993 at Kansas City. This latest meeting in Scotland is thus the second to be held outside the U.S.A. and the first to be held within the European Union. Over 45 participants from more than a dozen countries attended, along with an unusually large number of guests. Evidently its reputation for natural beauty, hospitality, and a romantic history made Scotland an attractive venue! For many this was their first visit, and nearly everyone took part in the full social program that had been designed to give at least a glimpse of the countryside, of some historic places, and of twentieth century life in the Scottish Highlands.

How successful the meeting was in overall terms, and what its ultimate impact will be, are matters for others to judge, but undoubtedly some exciting presentations were given, and (abbreviated) titles are listed here to give the flavor of the meeting.

On the first day, Monday July 10, the session on Concepts was opened by K. Mislow talking about *The Homochirality Problem*, and he was followed by E. V. Babaev (*Chemical Concepts/Surface Topology*); G. Gilat (*Structural Chirality*); D. Avnir (*Continuous Symmetry Measures*); R. B. Mallion (*The "Ring-Current" Concept towards the End of the Century*); M. H. Lee (*Polylogarithms and Statistical Thermodynamics*) and J. Cioslowski (*Atoms in Molecules and the Quantification of Chemical Concepts*).

Session II, on fuzzy logic, started with an authoritative general tutorial given by G. Klir, who followed this the next day with a masterly lecture entitled *From Classical Mathematics to Fuzzy Mathematics: Emergence of a New Paradigm for Theoretical Science.* Other contributors were D. H. Rouvray (*The Treatment of Uncertainty in the Physical Sciences*); F. M. Akeroyd (*Fuzzy Logic and the Hughes−Ingold Theory*); J. Xu (*Fuzzy Graphs in Chemical Research*); A. Amann (*Fuzzy Classical Structures in Genuine Quantum Systems*); P. Mezey (*Fuzzy Measures of Molecular Shape and Size*); and J. Brickmann (*Linguistic Variables and the Molecular Recognition Problem)*. This session, the first of its kind in chemistry, aroused considerable interest and discussion. There is no doubt that the chemical community is still divided on the relevance and usefulness of fuzzy logic. Some are enthusiastic proponents, while others tend either to deplore its inherent and accepted lack of rigor or to feel that it merely dresses up old "practical common sense" in pretentious new clothing. The idea here, however, was simply to introduce such ideas to the audience and let them make up their own minds.

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Following these sessions, the overt focus of the meeting returned to chemical concepts, gradually shading into general mathematical chemistry (in so far as such a discipline can be defined). The concept of aromaticity is an old and familiar one, and, however fuzzy its definition, it has inspired a huge wealth of fascinating research, both practical and theoretical. D. M. G. Lloyd emphasized this point when he asked *what is aromaticity*. Other papers were given by N. S. Greenspan (*Ontological Dynamics and Immune Recognition*); R. B. King (*Porous Delocalization in the Chemical Bonding Topology of Superconductors*); E. A. Smolenskii (*Topological Structure of the Configuration Space of Many Body Systems* and *The Pauli Principle and Nodal Surfaces of Wave Functions*); and D. J. Klein (*Similarity and Dissimilarity in Posets.*). H. Hosoya ventured into the fourth dimension in his chemistry (*Explore the 4-D World and Realize 3-D Chemistry Better*), while M. L. Ellzey discussed *Symmetry-Adapted Bases of Matrix Spaces Applied to Quantum Chemistry*. After this the meeting heard from A. Zeigarnik (*From Intuition to Mathematical Thinking*); T. Wieland (*Generation of Constitutional and Configurational Isomers*); T. A. Ford (*Ab initio MO Studies of Some Complexes of Boron Trifluoride*); J. R. Dias (*MO Functional Groups—Subspectrality of Polyene Molecules* and *Formula Periodic Tables and Related Symmetries*); A. Korobov (*Reacting Bertholide Compounds: The Loss of Certainty*—a poster presentation given in absentia); E. V. Babaev (*The Superconsonant Molecules: First Closed Subset in Chemistry?*); E. E. Daza (*Chemical Structure: A Concept Beyond the Born−Oppenheimer Approach*); J. J. Aranda (*Generators of Molecular Systems in the Nuclear Charge Space*); R. A. Hefferlin (*Molecular Multiplets of Alkaline Atoms* and *A More Rigorous Articulation of Small-Species Periodicity*); E. C. Kirby (*Fully Arenoid Toroidal Fullerenes*); M. Klin (*The Stabilization of Graphs*); I. Lukovits (*The Partition Coefficient in Terms of Graph Invariants*); S. S. Tratch (*Combinatorial Approach to Stereochemical Problems* and *Mathematical Models of Some Molecular Design Problems*); L. V. Quintas (*Progress and Problems on the Random f-Graph Process*); P. Hansen (*Enumeration of Trees by Reverse Search*); Y. Isu (*Neural Network Simulator for Structure−Activity Correlation of Molecules: NECO, and Applications*); J. Pospichal (*Construction of Molecular Graphs by Simulated Annealing*); and M. Razinger (*Molecular Shape and Chirality*).

A selection of these papers is presented here, together with some contributed by authors unable to attend in person. Most of the remaining papers are to be found in somewhat expanded form in two forthcoming books: *Fuzzy Logic in Chemistry* edited by D. H. Rouvray (Academic Press, San Diego) and *Chemical Concepts in Chemistry* edited by D. H. Rouvray and E. C. Kirby (Research Studies Press, Taunton, England UK).

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