

Proceedings of the “Mathematics in Chemistry Meeting”, Leipzig, Germany, October 26 - 28 2016

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In the early 1970s, Oskar E. Polansky (1919-1989), a leading theoretical chemist, started to show interest in graph theory and its relationship with chemistry [1]. As director of the Radiation Chemistry group at the “*Max-Planck-Institut für Kohlenforschung*” (MPI-KoFo) in Mülheim, he collaborated with several visiting scientists from the former Yugoslavia, Bulgaria and Romania, important countries for the 20th century connection between graph theory and chemistry [2]. In the context of this collaboration, he organised the micro-symposium “Graph theory in Chemistry” at the MPI-KoFo in May 1975. Beyond the scientific interchange, a lasting outcome of the meeting was the idea to create *MATCH Communications in Mathematical and in Computer Chemistry*¹ as the first printed channel to share results on the interface between mathematics and chemistry, a kind of research that initially was not readily accepted in mainstream theoretical chemistry [2].

¹Initially called *MATCH Informal Communications in Mathematical and in Computer Chemistry*.

With this historical connection between Mathematical Chemistry and the Max Planck Society in mind, the “Mathematics in Chemistry Meeting” was held at the Max Planck Institute for Mathematics in the Sciences (MPI-MIS) in Leipzig from October 26th to 28th 2016. The meeting gathered 21 speakers from 12 countries² and provided a balanced view of current mathematical approaches to chemistry, going beyond the initial historical and important ones from graph theory.

The meeting was supported by the MPI-MIS, the Alexander von Humboldt Foundation, and Leipzig University. The complete list of participants and lectures’ abstracts are available online³. Given the diversity of topics covered, a special issue of MATCH dedicated to the material presented in Leipzig seemed appropriate. The final outcome of the editorial process is the content of the present issue, which was entirely supported by the three mentioned institutions and which can be summarised and interrelated as follows:

Taking the molecular level of the chemical ontology as starting point, it is appropriate to begin with the paper by Kerber, who shows the historical chemical importance of enumerating molecular formulas and the mathematical challenges this question brings out.

Once having sets of molecules and even going further to the ontology of substances, one finds that a historical chemical question has been the assessment of similarity of its species. Here, Holliday, Sani and Willett discuss the case of molecular similarity and, particularly, show how molecular similarity scores based on genetic algorithms can be fused and contrasted with the simple genetic algorithms’ scores. The authors show that their fusion methods are superior than the simple scores.

As Holliday, Sani and Willett point out, description of molecules in a machine readable form is utterly important to run comparisons of molecules. Besides fingerprints encoding molecular fragments, discussed by the authors, other approaches focus on the graph representing the molecular structure. This led to the active field of molecular descriptors in mathematical chemistry [3, 4]; which is somehow synonym of mathematical chemistry, in spite of having several other approaches to chemistry not only related to discrete mathematics [5].

An interesting discussion on molecular descriptors was brought forward by Gutman,

²Austria, China, Colombia, Croatia, Denmark, Germany, Italy, Japan, Romania, Serbia, UK and USA.

³<https://sites.google.com/site/mpimsmathematicsinchemistry/home>

Editor-in-Chief of MATCH, who also gave a lecture at the meeting. He talked about the future of the rapid growing field of molecular structure descriptors. About these descriptors, other participants working in the field talked about the different ways to encode/decode information of the molecular graph.

The energetic difference between the HOMO and LUMO⁴, known as HOMO-LUMO gap, has been found to be related to the eigenvalues of the molecular graph. In fact, the gap is defined as the difference of two of those eigenvalues. In their paper Wu, Yang and Ye show that these eigenvalues, for bipartite graphs with at most one perfect matching, fall into a particular interval.

Vukičević, Li, Sedlar and Došlić, in turn, introduce a new topological index for molecular graphs that is only based on vertex degrees. They also discuss some of its mathematical properties for extremal graphs and trees and compare their index with some others.

Diudea, Pîrvan-Moldovan, Pop and Medeleanu report the energy of hypercubes, spongy hypercubes, propellanes and C₄₀ fullerenes, where the energy of the graph takes its usual definition as the sum of the absolute values of the eigenvalues of the adjacency matrix associated to the graph.

Related to the future of molecular descriptors, Hutchinson, Kamat, Larson, Mehta, Muncy and Van Cleemput present their scientific programme of computationally obtaining new descriptors and exploring their bounds. The algorithm is in particular applied to the domination number of benzenoids.

Bridging the ontological level of molecules with that of chemical reactions, Andersen, Flamm, Merkle and Stadler show that chemical reactions can be formalised through transformations of molecular graphs of educts into products. This is attained by using the formalism of graph rewrite rules, through the language of category theory, where morphisms are the key concepts relating molecular structures. In this approach, a chemical reaction is a transformation rule, which can be composed with other rules leading to new transformations.

As an application of the graph transformation rules, Andersen, Fagerberg, Flamm, Kianian, Merkle and Stadler show how the rules can be used to estimate mass spectra by modelling the fragmentation process undergone by chemical species. The algorithms for

⁴HOMO and LUMO stand for Highest Occupied and Lowest Unoccupied Molecular Orbital, respectively.

running the modelling are described.

Still at the ontological level of chemical reactions, but this time not regarding the internal structure of molecules, Stadler, Jost and Dittrich show their approaches to characterise networks of chemical reactions.

Bärbel and Peter Stadler explore the topological structure of spaces of substances related through chemical reactions. In so doing, they model a reaction as a bipartite hypergraph relating educts with reactions and reactions with products. These spaces are studied through closure functions which are further compared with other closure spaces showing the strong difference of the chemical ones.

Another approach to the structure of chemical reaction networks is brought out by Saucan, Samal, Weber and Jost, who develop an approach to the analysis of chemical reaction networks that is based on characteristics of edges rather than vertices. More concretely, they propose and evaluate an approach based on discrete notions of network curvature and explore its potential for identifying qualitative properties of such networks.

Dittrich and his team have defined molecular codes in chemical reaction networks as mappings from sets of educts to sets of products that require some other substances to occur. In their current contribution, Neu, Ibrahim and Dittrich report computational approaches and algorithms to identify those molecular codes. The implemented method is based on the algebraic properties of some sets of substances that form a lattice.

Some of the efforts to characterise chemical reaction networks are motivated by questions on the origin of life that look for chemical reactions of the prebiotic world able to evolve and give place to structured systems. In that direction, Schuster shows that evolution can be seen as a special case of chemical reaction networks containing either single autocatalytic reaction steps or subsets of reactions forming together an autocatalytic network. In his paper, the author presents a mathematical model for evolution based on three sorts of chemical processes: the competition of substances X_i s for an educt A in reactions $A + X_i \rightarrow 2X_i$, the symbiotic cooperation of X_i and X_j for A in reactions $A + X_i + X_j \rightarrow 2X_i + X_j$ and the variation through mutation in reactions $A + X_i + E \rightarrow X_j + X_i + E$, with E being another substance. The mathematical properties of these processes are explored by the author.

Brüggemann, Kerber and Restrepo take distance from the two mentioned ontologies of chemistry and move to the interaction of them with others, e.g. in cases of environmental

chemistry and biotechnology. These cases fall into the area of decision making, where decisions are characterised by n -tuples of decisions' attributes. Brüggemann and Carlsen criticize that, normally, the n -dimensional structure of the decisions is reduced to a single dimension through weighted linear combinations of the n -tuple. The authors then discuss the possibilities partial order theory offers to analyse these weights of the combinations and how the uncertainty on those weights is related to incomparabilities in the underlying partially ordered set.

Quintero, Brüggemann and Restrepo discuss the practical problem brought out by considering all n dimensions at once, which leads to multiple intersecting lines in the typical representation of the partially ordered set (poset) underlying the space of possible decisions. The authors introduce the posetic coordinates as a solution to map the poset into spaces of one and two dimensions. The mathematical properties of these mappings are explored in their contribution and applied to microorganisms used in uranium recovery.

Going beyond the evaluation of the n -dimensional space, Brüggemann and Kerber show the importance of analysing the n attributes in a process they call "exploration", where also elements of partial order theory can be used. The methods used come from lattice theory and are also discussed in the framework of Formal Concept Analysis.

The meeting and the papers here presented show that mathematical approaches to chemistry are diverse. We hope MATCH readership will take advantage of these new avenues of research.

References

- [1] K. Jug, *Die Gründungsphase der modernen Theoretischen Chemie aus der Chemie*, Springer, Berlin, 2015, pp. 31–54.
- [2] G. Restrepo, J. L. Villaveces, Discrete mathematical chemistry: social aspects of its emergence and reception, *HYLE* **19** (2013) 19–33.
- [3] G. Restrepo, P. Willett, A bibliometric profile of MATCH Communications in Mathematical and in Computer Chemistry, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 235–242.
- [4] G. Restrepo, P. Willett, The Journal of Mathematical Chemistry: A bibliometric profile, *J. Math. Chem.* **55** (2017) 1589–1596.
- [5] D. J. Klein, Mathematical chemistry! Is it? And if so, what is it? *HYLE* **19** (2013) 35–85.