

—CALL FOR PAPERS—

HYLE: International Journal for Philosophy of Chemistry
invites papers for a special issue on

Chemistry & Mathematics

Deadline: August 15, 2011

The relationship between mathematics and chemistry has a long history. In fact one of the new features of modern chemistry was the introduction of arithmetical relations by Lavoisier. One could even argue that the oldest molecular theory, in Plato's *Timaeus*, was a geometrical theory of chemistry. Not only chemistry but also mathematics has benefited from the relationship, as can be acknowledged in the development of Graph Theory, a mathematical theory with roots in chemical questions. Other important results from this synergy are related to symmetry, such as the conception of a tetrahedral carbon, the octahedral symmetry of certain coordination compounds, the hexagonal nature of benzene, or the interpretation of spectra, on the one hand, and the development of the mathematical theory of symmetry out of mineralogy, on the other. More recent examples of successful interplay between mathematics and chemistry include the understanding of fullerenes, the rational design of drugs, and the estimation of toxicological and environmental impact of chemical substances.

And yet, chemistry and mathematics could hardly be more different in methodological regard: a strict experimental science here and a purist a priori approach there. That difference was perhaps responsible for the comparatively small role that mathematics has played in chemistry compared to its role in physics. While such methodological tensions have been influential in mathematical physics since centuries, the field of mathematical chemistry has slowly emerged only since the 1970s. More recently it has established itself with an International Academy and an International Society of Mathematical Chemistry as well as two specialized journals, *MATCH Communications in Mathematical and in Computer Chemistry* and *Journal of Mathematical Chemistry*. The delayed development of mathematical chemistry suggests that there are considerable barriers between mathematics and chemistry, which philosophical analysis might help understand and perhaps eventually overcome.

Because HYLE is the international journal devoted to philosophy of chemistry, it is the ideal place for posing philosophical and historical questions regarding both the relationship between mathematics and chemistry and the nature of today's mathematical chemistry. We particularly welcome papers on one or more topics of the following non-exclusive list:

Philosophical foundations of mathematical chemistry

- Is mathematical chemistry a distinct field that can be clearly defined and distinguished from other established and related fields, such as physical chemistry, quantum chemistry, and mathematical physics?
- Does mathematical chemistry have a specific methodology and epistemology that distinguish it from both mainstream chemistry and mathematics as well as from mathematical physics?
- Does mathematical chemistry produce a priori or a posteriori knowledge? Is it a theoretical science as opposed to experimental chemistry? Could there be an experimental mathematical chemistry?

- Does mathematical chemistry require specific ontological or metaphysical assumptions or positions regarding the (mathematical) constitution of the world or the reality of mathematical entities?
- Are there specific branches of mathematics that are particularly appropriate for mathematical chemistry? If so, does that tell us something about chemistry in general and mathematical chemistry in particular?
- Does mathematical chemistry necessarily require or actually establish new relationships between mathematics and chemistry, other than taking mathematics as a mere tool for chemistry?
- Are there particular links between mathematical chemistry, on the one hand, and philosophy of chemistry and philosophy of mathematics, on the other?

History of the mathematics/chemistry relationship and mathematical chemistry

- Does the history of the chemistry/mathematics relationship provide any clues as to what has fostered and hindered its cooperative development?
- Why did mathematical chemistry emerge so late compared to mathematical physics?
- How did today’s mathematical chemistry actually emerge? What socio-cultural and cognitive factors favored its development and determined its current shape and research focus? How was the development received by mainstream chemistry and mainstream mathematics?
- Could mathematical chemistry have been differently developed under different historical conditions? Could there be other definitions, other main areas, or even other methodologies and epistemologies of mathematical chemistry?
- Did the development of mathematical chemistry have any impact on other branches of chemistry and mathematics or even beyond?

Manuscripts should follow the general Guidelines for Authors, available on the HYLE website (www.hyle.org). Send inquiries regarding the suitability of submissions etc. and your submission in appropriate form for anonymous reviews not later than August 15, 2011 to

Guillermo Restrepo, Guest Editor

Laboratorio de Química Teórica, Universidad de Pamplona, Pamplona, Colombia; grestrepo@unipamplona.edu.co, and guillermorestrepo@gmail.com

Or to

Joachim Schummer, Editor-in-chief of HYLE; mailto:editor@hyle.org