Special Anniversary Issue

MODELS IN CHEMISTRY (1)

Editorial

It is my pleasure to open this special issue with which we like to celebrate the fifth birthday of our journal. What was originally conceived as one special issue of HYLE that has rapidly grown to a considerable number of high quality papers for which we need at least two issues. We received a total of 19 paper submissions, some of which are still under review. The manuscripts cover nearly every aspect of models outlined in the Call for Paper (HYLE 4, pp. 171f.), and much more. As far as the review procedure allows, we are going to divide the topic roughly into three topical sections, each with about four contributions. The following four papers of the present volume make up the first section that is devoted to models in quantum and computational chemistry. The second section, to be published in the next issue, is more specifically on a very peculiar type of models in chemistry: molecular models. The third and last section will be on models of complex systems, in particular in biochemistry, geochemistry, and chemical engineering.

We are happy to begin the special issue with a fine series of papers both from two chemists and two philosophers, all well-known from their previous publications on models in chemistry. The introductory part is taken by the outstanding Italian theoretical chemists JACOPO TOMASI. Against the background of a broad survey of the history of theoretical chemistry from the early 19th century until today, he argues in detail for methodologically reflected and chemically adapted standards for models that are used to design and to interpret quantum chemical calculations. While Tomasi excludes the metaphysical issue of reductionism to confine his approach to methodological issues proper, British philosopher ROBIN F. HENDRY addresses the complementary question whether the explanatory success of quantum chemical models supports physicalism. His detailed analysis, both of the concept of physicalism and the peculiar way molecular models are used in explanations, leads to a negative answer, since a basic claim of all kinds of physicalism, the completeness of physics, appears to be ignored in typical cases of successful explanations.

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The second couple of papers deal with recent computational approaches in chemistry. German philosopher KLAUS MAINZER, also known from his former article on 'Symmetry and Complexity' (HYLE 3), gives us a condensed outline of chemistry's various mathematical and computational ways of modeling molecules – from the past to the near future. Starting with topology, graph theory, and classical quantum chemistry, he presents recent trends in computer aided molecular design, object-oriented programming for 3D molecular structures *etc*., and discusses perspectives on future chemical research, such as the replacement of experiments by computer simulations and new forms of collaborative research on the World Wide Web. As a kind of counterpart, US chemists CARL TRINDLE looks upon recent trends of computer modeling in chemistry from the perspective of graduate students (and their adviser) in two case studies. His 'Entering Modeling Space' is at first an astute analysis of expectations, frustrations, and actual success that chemists experience when first using the new computational devices. The psychological account then turns into a critical methodological evaluation of computational models, based on criteria developed in a former paper.

Without doubt, the 'model topic' has attracted new attention to the philosophy of chemistry from various sides, and the interest will grow in the course of the publication of this and the next issue. Despite the many meanings of the term, the scientific notion of models invites both scientists and philosophers of science for epistemological and methodological reflection, because models, in any scientific meaning, are at the interface between our conceptual world and the objects of empirical investigation. The inherent tension of models seems to be that, while they are certainly more on the conceptual side such that we need to put rational constraints on their production, we are nonetheless inclined to identify their exact counterparts on the other side. That is why models are central both to science and philosophy of science, and in particular to philosophy of chemistry.

Notwithstanding the epistemological significance of the topic, there are many other important issues in philosophy of chemistry waiting for exploration. Occasionally, we will invite papers for further special issues of HYLE. For the time being however, we would like to reinforce our general CALL FOR PAPERS on any philosophical aspect of chemistry.

Due to the strict schedule and the extraordinary amount of submissions, a special issue requires extra efforts by all participating referees. Finally, I would like to thank all of them for their competent advice and their discipline.

Joachim Schummer