Special Anniversary Issue

MODELS IN CHEMISTRY

(2) 'Molecular Models'

Editorial

As supposed in the last Editorial (HYLE 5-1), our special topic 'Models in Chemistry' has attracted new attention to the philosophy of chemistry. Only during the past couple of month, the number of visitors of the HYLE website has nearly doubled to some 1,600 per month. There is nothing comparable in the whole field of philosophy of science, as there is no other science having such a lot to catch up on philosophical work. At the same time, this means a great challenge to meet the expectation of such a large and heterogeneous readership.

I am very confident that the present issue comes up to all these expectations. In particular, chemists will find a wealth of astute reflections on their favorite objects, molecular models. Philosophers of science, while being usually occupied with either mechanical models in the Maxwell tradition or so-called 'models' of formal semantics, may learn more about the various uses of models in science. In addition, historians of chemistry will benefit from two epistemological analyses of the uses of models in the history of stereochemistry.

The present section on molecular models consists of 5 papers, grouped in two pairs and one very special contribution. The first couple of papers present different epistemological approaches to models of molecular structure. Italian theoretical chemists and philosopher Giuseppe Del Re has taken the introductory part. He discusses how both analogies to everyday objects and idealizations are applied to built models as means for the understanding of different complexity levels of reality. Molecular spring-and-ball models exemplarily prove the usefulness of that approach. Following his former paper on 'The Ontological Status of Molecular Structure' (HYLE, **4**, pp. 81-103), he shows how the resulting analogy models of molecular structure are reconciled with quantum chemistry.

Against the background of recent debates in philosophy of science on the realism vs. instrumentalism issue, Polish philosopher Paweł Zeidler critically analyzes if models of molecular structure fulfil a representational function at all. He argues that the classical notion of rigid molecular structure is neither

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free of theoretical idealizations nor independent of certain experimental contexts, such that a rigid molecular structure can hardly be something real to be represented. By comparing rigid models with the more sophisticated dynamical models of molecular structure, he suggests that, rather than being representations of structures, they fulfil only informational functions for chemical purposes.

The second couple of papers, authored by two temporary research colleagues at the Max-Planck-Institute for the History of Science, explore the uses of and the epistemological attitudes towards molecular models in crucial episodes of the history of stereochemistry. Both results may easily be transferred to present day chemistry. U.S. historian of chemistry Peter J. Ramberg asks how early stereochemists, from van't Hoff to Werner, coped with the fact that their stereochemical models had implication about the structure of atoms that were incomprehensible by the laws of physics. He argues that the main attitude of stereochemists was simply to ignore these implications and consider the molecular models in a pragmatic way for chemical purposes and contexts only. Other chemists, who believed in physicalistic reduction, developed atomic models in order to reconcile the physical and the chemical view in some sense, without being really reductive, however, nor having much impact on chemical practice and theory.

Canadian sociologist and historian of chemistry Eric Francoeur raises the question why chemists are fond of using material models of molecules, instead of graphical formulas. In two case studies on conformational analysis in stereochemistry, he shows how material models became the objects of chemical investigation rather than being mere representations. Beyond illustration and inscription, material models served to derive new concepts and were subjected to manipulation and measurement. Once some basic information had been materially stored in the model components, chemists were even able to derive new data from the models, in a way "akin to an analogic computer".

Chemists' specific affinity to molecular models even goes much further as the final contribution to this section proves. Belgian organic chemists Pierre Laszlo, also known from his 'Chemical Analysis as Dematerialization' (HYLE **4**, pp. 29-38), explores the uses of models at the interstice between epistemology and depth psychology. By carefully analyzing the psychological features of playing and toys, he argues that chemists attitude towards molecular models exactly reflects all these features. Among a wealth of interesting aspects, his psychological approach also reveals the epistemic side of manipulating molecular models as a kind of playful testing of hypotheses. "To the professional chemist," Laszlo concludes, "molecular models are as much toys as they are tools."

Enjoy reading!

Joachim Schummer, Editor