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EDITORIAL 12

The final issue of volume 4 contains a mixed-bag of articles. It begins with a paper on emergence in chemistry, written by Pier Luigi Luisi who is a world expert on the scientific origins of life. Of course the emergence of life from inorganic chemical compounds represents the most dramatic example of emergence one could imagine but this is not the main topic of the current article even if this question may have served as a major motivation for the author.

Instead Luisi goes to some lengths to consider the main forms of emergence that have been discussed in the literature, such as strong and weak emergence, and he suggests that the best place to study emergence is chemistry. For example, he points to the properties of water, such as its liquidity, that emerge following the chemical combination of the gases oxygen and hydrogen that have quite different properties.

The question of emergence is quite frequently mentioned alongside that of reduction since in some ways it represents the opposite process, but of the two questions emergence has received far less attention in the literature.¹ Luisi's article dealing specifically with emergence in chemistry is therefore a welcome addition to the renewed interest in the philosophical aspects of chemistry. One might also connect these discussions on emergence with the studies that have raised the question of how, if at all, the elements survive in the course of compound formation. This complimentary question is the topic of an important paper in philosophy of chemistry by Paneth which appeared many years ago (Paneth, 1962).²

The second article, by Mark Eberhart, is a provocative attack on common wisdom regarding the application of computational chemistry to the synthesis of new molecules and materials. The author suggests that just as the phlogiston theory once delayed the development of chemistry, so the present views about different bonding types are delaying the full benefits of computational quantum chem-



istry in the field of chemical synthesis. Eberhart claims that “[r]ather than providing a new representation of the chemical bond, quantum mechanics became the mirror through which the old bond was reflected. . . . By the 1950s, molecules were described in terms of a veritable zoo of different bond types.” His arguments are illustrated by specific examples such as transition-metal carbides as well as nitrides and also nickel-aluminum alloys where there is still disagreement about the precise nature of the bonding that exists between the atoms concerned. Finally he briefly suggests some new indicators of bond types that are related to measures of charge density obtained computationally.

The third and final full-length article is written by Justi and Gilbert, two chemical educators who for some time have explored the notion of chemical models in relation to the teaching of chemistry. The present study presents the findings of a series of interviews aimed at probing the views of U.K. and Brazilian educators on the nature and role of chemical models. Rosária Justi and John Gilbert interpret their findings to mean that the teaching of models is still being carried out in a traditional manner and that teachers frequently fail to introduce or explicitly address the nature of models.

The issue comes to a close with a highly detailed book review, by our own book review editor, John Bloor, of Gillespie and Popelier’s recent volume on chemical bonding and molecular geometry. Bloor who began as an organic chemist but then turned to computational chemistry provides a very sure-footed guide to this book and to recent developments in such areas as VSEPR. Coincidentally VSEPR, which has now even permeated the under-graduate chemistry curriculum, was initiated by one of the authors of the book under review, Ronald Gillespie. As in the case of Eberhart’s article the aim of Gillespie and Popelier’s book is to go well beyond just computing atomic and molecular properties but to make detailed connections between calculations and the chemist’s central paradigm of structure and bonding. Bloor’s review gives the reader the necessary context and background to appreciate the wider aspects of this work while also maintaining a critical eye. This is a model of what a book review should be like and I hope that Bloor’s efforts will encourage other readers to offer their expertise in reviewing books in a similar manner for this journal.³

Returning to the book under review, the theoretical background for this book is provided by the extensive research of Richard Bader who has pioneered a technique that he calls Atoms in Molecules or AIMS.^{4,5} It is a little surprising that we have yet to feature a philosophical discussion of Bader's rather unique approach to quantum chemistry in this journal and I personally would welcome receiving a submission along these lines from any interested parties.

Finally, I would like to quote an interesting line from a physicist writing in one of our Kluwer sister journals, *Foundations of Physics*.

This article presents arguments in support of the view that both the standard model of elementary particle physics and general relativity are preconditions of an "interesting" world, defined by Squires as one that contains chemistry. (Mohrhoff, 2002)

How odd that most of philosophy of science carried out up to this point should have been based on what is presumably the less interesting world of physics!⁶

NOTES

1. Some previous studies on emergence that at least mention chemistry are by Paul Humphreys as well as a very recent article by Kronz and Tiehen and some edited collections based on conferences organized by Achim Müller (Humphreys, 1997; Kronz and Tiehen, 2002; Mainzer, Müller and Salzer, 1998).
2. This article has recently been re-examined and an attempt has been made to apply Paneth's views regarding an "intermediate position" to modern chemistry (Scerri, 2000).
3. Readers interested in reviewing any recent books of a similar general chemical appeal are invited to contact John Bloor directly.
4. Bader too began as an organic chemist but later turned to theoretical chemistry.
5. A short introduction to Gillespie's approach appears in a recent article in the *Journal of Chemical Education* (Matta and Gillespie, 2002).
6. The reference is to Squires (1981).

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