ERIC R. SCERRI

EDITORIAL 4

Since the appearance of the last issue of this journal reports have been published in several science magazines, which if correct, might threaten to shake the very 'foundations of chemistry'. Rightly or wrongly, modern chemistry, at all levels, is underwritten by quantum mechanics. Among chemists this connection with theory is often maintained rather remotely by appeal to atomic and molecular orbitals. Whereas theoreticians regard these entities as being mere mathematical constructs, devoid of any physical significance, people in all other areas of chemistry as well as chemical education tend to adopt an approach which favors the visualization of orbitals. As a result of such visualization, which is of course one of the main ways that chemists operate successfully, the physical existence of orbitals is sometimes wrongly entertained in that the model is confused with reality.

A dramatic illustration of these pitfalls has recently been provided by the reports, featured on the front cover of the prestigious magazine 'Nature', among many other science magazines,[1] to the effect that 'textbook orbitals' have been directly observed for the first time (Zuo et al., 1999). This claim is patently nonsense, just as the infamous claim made about a decade ago to the effect that nuclear fusion had been achieved at room temperature in a test tube. Of course I will not now provide a detailed argument for why the claims to having produced direct images of orbitals are necessarily incorrect, since an Editorial is not the place for such an exposition. Such analyses are bound to be published in the months to come, quite probably in future issues of this journal.

In the case of cold fusion the authors were much criticized, among other things, for making the preliminary announcement at a press conference rather than through the medium of peer reviewed journals. The claims for the sighting of orbitals cannot be faulted

Foundations of Chemistry **2:** 1–4, 2000.

on this criterion. The primary article appeared, as mentioned above, in the pages of the world's leading scientific news journal, known for first announcing the discovery of the electron, pulsars and the structure of DNA to name but a few scientific landmarks. In addition, the article was the feature of an Editorial, presumably by an expert in the field who extended the claims made by the primary researchers and emphasized the notion that the pictured orbitals were the same as those featured in so many chemistry and physics textbooks (Humphreys, 1999).

Admittedly, the primary authors stop just short of making the categorical claim to having definitely observed orbitals, by only pointing out the remarkable resemblance between textbook orbitals and the images they obtained. Clearly, what the images represent is not orbitals but electron density, and not for the first time either. However, in spite of the flood of criticism and discussion which has taken place on various Internet discussion lists, following the wake of the announcement, the primary authors have refused to distance themselves from the claimed reports of 'textbook orbitals observed'. I cannot but conclude that in spite of the journalistic excesses which we have witnessed, part of the blame for what I will call this 'orbital hype' must lie with the primary authors themselves.

And now to the contents of this present issue. The first article is by Davis Baird, presently a senior research fellow at the Dibner Institute in Boston, and one of the leading historians and philosophers of chemical instrumentation. He is part of an evolving tradition among epistemologists who are outgrowing the view that knowledge is merely justified, true belief. Here Baird reviews some historical episodes in the development of spectrometers and discusses the relationship between the kind of knowledge obtained through instruments and through propositions in terms of Popper's World 1 and World 3, respectively.

History and philosophy of science have had something of an 'on-off' relationship ever since these fields began to be studied. If we consider the work of authors like Whewell and Duhem, we find an intimate connection between history and philosophy. However, the turn towards analytical philosophy led to the denial of historical aspects in the analysis of scientific developments. As is well known, the pendulum swung back again following the publications by

Kuhn, Feyerabend, Lakatos and other historically inclined scholars of science in the 1960s and 1970s. But more recently the divorce between historical and philosophical studies of science has established itself yet again. Few historians of science believe that there are general lessons to be learned from the historical unfoldment of scientific events, while many philosophers believe that they can make progress without getting too enmeshed in historical details.

John McEvoy is nominally in a philosophy department but, as his article in this issue shows, he is equally interested in the historical aspects of his area of specialty, namely the chemical revolution. This is perhaps the only area which was well represented during the years when it was considered unfashionable to study the central science of chemistry. McEvoy's paper presents an excellent summary of previous scholarship in the field as well as presenting his own insights.

The next piece is a commentary by one of the giants of computational quantum chemistry, Robert Nesbet, commenting on some of my own writings on quantum mechanics and the periodic system, as reported in an interesting article on philosophy of chemistry which appeared in 'New Scientist'. I hope that such dialogues with practitioners, from all areas of chemistry, might become a regular feature of this journal.

Finally, we present a review of Joachim Schummer's book, which, rather surprisingly perhaps, is the only single-authored, full-length book on philosophy of chemistry to appear since the re-emergence of the field in the early 1990s. This book, which unfortunately is not yet available in an English translation, is reviewed in some detail by Jeffrey Ramsey, a philosopher who has established a reputation with his analysis of the molecular structure controversy and other chemical topics such as the study of rates of reactions (Ramsey, 1997).

NOTE

1. The other magazines have included Physics Today, Chemical & Engineering News and Science, as well as the New York Times. In addition, the Internet Supplement of Scientific American has featured the story on two separate occasions.

REFERENCES

C.J. Humphreys. Electrons Seen in Orbit. *Nature* 401: 21–22, 1999.

J. Ramsey. Molecular Shape, Reduction, Explanation and Approximate Concepts. *Synthese* 111: 233–251, 1997.

J.M. Zuo, M. Kim, M. O'Keeffe and J.C.H. Spence. Direct Observation of D-Orbital Holes and Cu-Cu Bonding in Cu_2O. *Nature* 401: 49–52, 1999.

Department of Chemistry,
Purdue University,
West Lafayette, IN 47907,
U.S.A.
E-mail: scerri@purdue.edu