COMMENTS ON:

"Can we Reduce Chemistry to Physics?"
Hans, Primas, Swiss Federal Technical School,
Zurich, Switzerland

by:
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I consider the paper by H. Primas on the relation between Chemistry and Physics very interesting and thought provoking, but I also find it very difficult to accept his main line of thought, although his espistemological analysis of quantum theory is well taken.

In his opening paragraph (p. 1) Primas equates the reduction of Chemistry to Physics to the reduction of Chemistry to Quantum Mechanics. This is not correct since neither is it correct to say that Quantum Mechanics is Physics or that Physics is Quantum Mechanics. The fact is that Quantum Mechanics is simply a formalism or theoretical construct to analyze, very successfully indeed, the basic properties of matter. Thus it does not make sense to talk of the "reduction" of Chemistry to Quantum Mechanics.

It also does not make much sense to talk any more about the reduction of Chemistry to Physics. Rather what we may say is that the two sciences are closely related or perhaps complementary, using the same basic principles (such as energy conservation) and dealing with processes involving matter (assumed composed of operational structures designated as particles, nuclei, atoms, molecules, etc.) and energy exchanges (such as radiation), assuming the same set of interactions (particularly electromagnetic and nuclear), and utilizing the same formalism (quantum mechanics). In fact what has occurred in the last 50 years or so is the development of a coherent or unified theory of matter and radiation, which serves as the common basis for the traditional sciences of Physics and Chemistry, each one dealing with particular types of phenomena but with strong overlaps. The best proof of this last fact is that Primas is Professor of "Physical-Chemistry." This is why I do not understand how Primas can say (p. 6) that "the concept of molecular structure is a classical idea foreign to traditional quantum mechanics." Again Quantum Mechanics is simply a formalism used to analyze molecular structure.

A quite different question is whether Quantum Mechanics is the "perfect" or "ultimate" theory to describe the behaviour of matter and energy. Nobody can be so arrogant as to assume so, but so far it is a quite "satisfactory" formalism. On the other hand we all recognize certain theoretical and philosophical problems associated with Quantum Theory. Two of these difficulties are Bohr's complementarity and Einstein, Podolsky and Rosen analysis of objective reality and separability, both analyzed by Primas, but that would be difficult to deal with them in more detail in this short note. However, neither of these concepts has much to do with "traditional" Chemistry. I will only say that I believe it is very difficult to renounce a certain degree of objective reality at the fundamental level and that we must not confuse objective reality with the way we find out about it through the process of measurement. Also, the relation between the concept of separability and the holistic approach implicit in Quantum Mechanics is a matter that requires a good deal of additional analysis and thought, but is essentially a philosophical question, rather that pertaining to the realm of Chemistry, or even to Physics.

I will refer now to some specific points related to Chemistry discussed by Primas. The first is the concept of valency and the affirmation that "to this day there is no theory of valency," and that "it makes no sense to say, for example, that the theory of valence by Heitler and London has reduced the concept of valency to quantum mechanics." I am very surprised of such statements by Primas. The initial concept of valency, as introduced in the early 20th Century, has become obsolete and has evolved into a broader and generally satisfactory understanding of chemical bonds. Once we recognize that atoms are composed of electrically charged particles obeying the rules of quantum mechanics, it has become relatively simple the explanation of stable polyatomic systems (ions, molecules, solids) using the properties of electromagnetic interactions and the formalism of Quantum Mechanics. But of course, that does not mean reducing valency to Quantum Mechanics, and nobody has ever made such a claim, which obviously is conceptually incorrect.

Primas affirms that "chemical systems are typically partly quantal and partly classical," (p. 6). Although the same could be applied to some physical systems (such as gases or solids or the motion of electrons in a TV tube), the statement itself is not correct. Whether we use a quantal or a classical analysis of a system depends on the nature of the system (one particle, few particles, many particles), the kind of properties being considered (pressure, dielectric permitivity, emission or absorption of radiation, etc.) and the degree of approximation needed. This is why I do not understand statements such as that "keto groups play an important role in chemical taxonomy, but this concept has no natural place in the framework of traditional quantum mechanics" (p. 18). In this statement Primas is again mixing apples and oranges . Besides, using elementary quantum mechanics it is relatively simple to explain keto-enol tautomerism. Similarly, I am amazed by the statement (p. 23) that while "the shape of molecules is an all important concept in Chemistry and in Molecular Biology, it is a classical concept which has no place in traditional Quantum Mechanics." I find hard to believe that Primas has never heard how, using Quantum Mechanics, one can explain that CO_2 is a linear molecule, H_2O is bent with an angle a bit larger than 90^o, NH_3 is pyramidal, and C_6H_6 is a plane hexagon.

Another topic dealt with by Primas and with which I do not agree is the relation between thermodynamics and statistical mechanics (p. 7, 8, 20). There is no doubt that classical Thermodynamics is a monumental theory, developed in the second half of the 19th century by intellectual giants such as Joule, Mayer, Helmholtz, Boltzmann, Kelvin, Maxwell and Gibbs, at a time when the structure of matter was not well understood. Although classical Thermodynamics is a very successful, elegant and formal discipline, it is essentially empirical and macroscopic, developed to describe the behaviour of matter in bulk. As time evolved and the structure of matter became gradually better understood, it was clearly recognized by Boltzmann, Maxwell, Gibbs and many others that it was necessary to relate the classical thermodynamcal concepts with the molecular structure and properties of the systems involved and thus emerged what is called statistical mechanics or statistical thermodynamics, or perhaps even better "molecular thermodynamics."

Certainly "thermodynamics is not the same as statistical mechanics" (p. 8). Rather both stand at opposite extremes in the description of the behaviour of complex many-particles systems: the micro-and the macro-descriptions, with statistical mechanics providing the molecular basis for explaining classical thermodynamics concepts (pressure, temperature, internal energy, entropy, heat capacity, etc.). The two methods of analyzing processes occurring in matter, rather than being mutually exlusive are complementary, and each science is valid in its own domain.

There are other aspects in Primas paper that deserve comments, but the above discussion is sufficient to indicate a fundamental disagreement with the way the author uses the term "quantum mechanics" and his interpretation of its applicability to explain "chemical phenomena."

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