COMMENTARY

The end of the dream of unity

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The dream of the logical–positivism at the beginning of the 20th century was the unity of sciences, according to which all scientific disciplines could be explained by means of the laws of fundamental physics. In this reductionist context, physics was at the top in the hierarchy of natural sciences due to its fundamental character whereas chemistry was relegated to an inferior position to the extent that it was supposedly derived from quantum physics. However, at the beginning of this century it is possible to stress that chemistry is neither a reduced science nor a branch of physics.

Is it possible to understand the behaviour of complex molecules and their reactions from the few laws concerning their atomic constituents? Could the whole chemical world be reconstructed from those laws? Reductionism has been a successful strategy to get knowledge: the explanation of complex systems from their component units was the traditional approach in the history of science. This approach led to attempts at reducing each special science to a more fundamental one: psychology to biology, biology to chemistry and chemistry to physics, specifically, to the laws of elementary particle physics. This reductionist view is rooted in the dream of the unity of sciences held by the logical–positivistic thought at the beginning of the 20th century: in the hierarchy of natural sciences, physics was at the top due to its fundamental character, whereas chemistry was relegated to an inferior position to the extent that it was supposedly derivable from fundamental physical laws.

As is well known, the advent of quantum mechanics produced a deep revolution in a wide variety of sciences including chemistry. The accuracy of the theory permitted one to understand many chemical phenomena, such as chemical reactivity, the nature of valency and the periodic table of the elements among others, from a new theoretical framework. The impressive success of quantum mechanics strengthened the traditional reductionistic view and led many physicists and quantum chemists to assume that chemistry can be completely reduced to the laws of fundamental physics. A famous statement of Dirac became commonplace in this line of thought: 'The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry [are] completely known from quantum mechanics'[1]. Dirac's views rapidly spread out, being propagated by many distinguished physicists and philosophers of science[2–5]: the epistemological reduction of chemistry to physics turned out to be a foregone conclusion. From this perspective, chemistry is conceived as a branch of physics or a secondary science, to the extent that it deals with complex systems (chemical systems) or particular processes which, nevertheless, could 'in principle' be described and explained by means of quantum theory. Whereas physics turns out to be a 'fundamental science' that explains nature in its deepest aspects, chemistry is considered as a mere 'phenomenological' discipline that only describes phenomena as they appear to us.

In recent years, a new generation of chemists and philosophers of chemistry has focused efforts on rejecting the alleged epistemological reduction of chemistry to physics. Several authors have stressed that quantum-mechanical approaches cannot compute the exact configuration of atoms that determine the chemical properties and, therefore, the place of each element in the periodic table; in other words, *ab initio* methods cannot fully deduce the details of the periodic table[6]. This means that, in general, the properties of a chemical system cannot be explained in terms of the properties of its physical micro-components; and even when the properties of a chemical macrosystem can be derived from those micro-components, this requires additional assumptions related with macroscopic phenomena (for instance, equilibrium in non-ideal multicomponent systems)[7]. In this context, the autonomy of chemistry is defended on the basis of the failure of epistemological reduction: not all chemical concepts and laws can be derived from physics; in particular, many relevant chemical notions, such as chemical bond, chirality or molecular shape among others, are not amenable to rigorous quantum-mechanical treatment[8]. Nevertheless, ontological reduction is taken for granted: chemical entities are, when analysed in-depth, no more than physical entities. In other words, the ontological dependence of the chemical world on the physical world is usually presented as a thesis which does not need to be discussed. This new perspective guarantees the methodological autonomy of chemistry with respect to physics, since it provides chemistry with a realm of specific concepts that have no place in fundamental physics. However, a new question arises: Is the mere failure of epistemological reduction sufficient for rejecting the secondary position of chemistry with respect to physics? When the ontological reduction of the chemical world is not questioned, the fundamental physical entities become the only 'real' entities and all the chemical concepts not derivable from quantum mechanics lose their referring character.

More recently, some attempts have been directed at reversing the secondary character of chemistry by appealing to symmetrical relations between the discourses of chemistry and physics[9] or to autonomous though related levels of reality[10]. In particular, it has been argued that the rejection of the traditional hierarchy of natural sciences requires one to abandon not only epistemological reduction, but also ontological reduction[11]. This position is based on an ontological pluralism, according to which the privileged viewpoint of God's Eye does not exist: we have access to reality only through our theories and, therefore, each theory constitutes a relative ontology when it cuts its own entities and properties out of the same substratum. According to this non-reductive view, we live in a diversified reality where different but equally objective theory-dependent levels of reality may coexist. Since the ontology of chemistry is as theory-dependent as quantum ontology, both have the same degree of 'reality': the chemical world does not depend on a more fundamental level of reality, but only on the theoretical framework that constitutes it. As a consequence, chemical concepts and properties like composition, bonding, molecular shape or chirality do not need yet to be referred to physical concepts and properties in order to acquire legitimacy as 'real': they are concepts and properties belonging to the chemical world, and their objectivity does not depend on the possibility of being referred to the supposedly more basic properties of physics. The fact that the description of a complex system requires qualitatively different laws from those that govern its units[12–14], turns out to be a natural consequence from this non-reductive perspective.

At present, one of the most discussed cases in the foundations of chemistry is about the interpretation of the concept of orbital. This case is an example of how philosophical questions have deep repercussions on the chemical sciences. As is well-known[15], the observability of atomic orbitals was spectacularly announced in 1999. Of course, the impact of this news rapidly pervaded the scientific community[16]. However, some authors immediately started a debate by claiming that interpretation of the experimental results was conceptually wrong[17,18]. Since quantum mechanics only includes the concept of wave function, the concept of orbital is deprived of reference in the real world. Therefore, it is not possible to obtain the image non-inexistent entity.

Although this interpretation was rapidly accepted by the authors of the experiment[19], a new announcement about visualization of orbitals was made later[20]. It is worth stressing that with this case, we are not simply facing a semantic problem but an ontological one. Indeed, the concept of orbital is key to education in chemistry: it is used to explain bonding, chemical structure and reactivity. Therefore, chemistry teachers naturally accept orbitals as real entities existing in the world. But their realist position clashes with the assumption according to which we have to follow quantum mechanics, i.e. only the concept of wave function is legitimate; the term 'orbital' has no reference in the real world.

With the purpose of solving this serious conceptual problem, some philosophers of chemistry have recently proposed well-founded philosophical frameworks[21–23]. These non-reductionistic interpretations of the concept of orbitals take into account the natural realism of chemists and chemistry teachers. In this sense, this pluralistic perspective allows us to use the concept of atomic orbital in chemistry in a realistic way, laying aside the pronouncements of fundamental physics. Thus, it is possible to speak about atomic orbitals in chemical ontology and about wave functions in quantum-mechanical ontology without contradiction between different levels of reality.

It is well known that quantum mechanics is one of the most successful theories in the history of science: its usefulness and predictive power cannot be denied. But, as in the case of biology[24], the limitations of the reductionistic programme in chemical sciences have been widely admitted. Chemistry is not a branch of physics nor a secondary science. It studies an autonomous realm of phenomena and, therefore, occupies the same hierarchical position as physics in the context of natural sciences. Perhaps it is time that physicists and chemists pay attention to the pronouncements of philosophers of chemistry about the old and complex issue of reduction: this would allow them to realize that it is possible to make profits by working together.

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ACKNOWLEDGEMENTS. We thank Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), of the Agencia Nacional de Promoción Científica y Tecnológica, of the Universidad del Centro Educativo Latinoamericano and of the Universidad Nacional de Quilmes, Argentina for grants.

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