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ON THE SPECIFICITY OF CHEMICAL EXPLANATION

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Summary

It is suggested that the view which considers the approach of chemistry reducible to that of physics is not correct. Chemistry explains the properties of materials in terms of special entities, the molecules: hence, in its descent toward the extremely small, it stops at a certain level of complexity, and adopts an "ontological" point of view; which implies the introduction of unique structural concepts, such as the chemical bond. Historical considerations confirm the view that chemistry is complementary to physics. Physics proper retains a special status insofar as it seeks explanations in terms of motion governed by first principles; but by the same token it provides only partial answers to scientific inquiries.

Scientific explanation and reductionism

According to the project of reductionism in the physicalists'version, observed facts are explained when they are traced back to the concepts and laws of physics. If this project is practicable, then there is no such thing as a "chemical explanation", and a model like the well-known nomological-deductive one of Hempel and Oppenheim |2| does apply. In other words, an "explanans" is just a set of general laws and of given initial conditions, no special role being assigned to the entities entering a given phenomenon. Those entities have been traditionally assumed to be the ultimate constituents of matter. Indeed, in spite of the increasing number of elementary particles and of the complications of nuclear physics, even today the programme of physics is consistent with the old scheme, as is witnessed by recent developments in the quark hypothesis; it tends to trace all phenomena back to a single type of "elementary" particle.

The reductionist dogma lies behind the prevailing trend of present "Quantum Chemistry", which has in fact evolved into the so-called "Computational Chemistry": here the basic tenet is that all of chemistry is contained in the Schroedinger Equation. The latter is supposed to "explain" chemistry in terms of the properties of nuclei and electrons. In the view of many chemists, this has led to an increasing separation between quantum chemistry and theoretical chemistry, viz. the part of chemistry which lies beyond the mere description of facts and the prescriptions fro preparing the various compounds.

This situation, as well as the developments which have shown the impossibility of reducing biology to physics, have made actual again a discussion of the specificity of chemistry and of chemical explanation.

Ontological explanation and complexity

A few studies bearing on this question have appeared in recent years. We recall in particular an article by M.Levy |3| , who showed that the physicalist dream, even granting that it can become true, could do so only on the condition that physics be extended to include concepts which are at present outside it. An important example is the chemical bonds.

The contention of this paper is that even the extension of physics to include more concepts would not suffice to reduce chemistry to it. The ground for this claim is that chemistry has been led hystorically to introduce special concepts because it views reality from a perspective different from that of physics,and deals with a different level of it. The question "why" is understood by chemists in a specific way, and thus chemical explanation has its own scientific status.

Key terms apt to characterize it are probably "ontological" and "complexity". Like physics and biology, chemistry starts from the macroscopic level, and proceeds in what Halbwachs would have called a bathogenous direction |1| . In thus reaches a microscopic level of complexity where concepts like "living" no longer apply, but the number of different entities which can be made responsible for the properties of matter is high enough (say, 90 or so) to provide combinations (the molecules) accounting for the macroscopic facts to be "explained".

Consider a question such as: way is grass green? Physics answers: because it absorbs red light; chemistry answers: because it contains chlorophyll. This example lends itself to a very extensive discussion of reductionism and of interplay between different disciplines. Here it illustrates what we have called the "ontological approach of chemistry: the question "why?" is answered by indicating - at least in the first instance - the entity which is responsible for the "explanandum" at the molecular level,viz. at the level of complexity where chemistry stops its bathogenous plunge. The next step may well be to explain why chlotophyll absorb in the red region of the visible spectrum; but again, even though it may make use of concepts of physics, chemistry will try to emphasize the role of molecular structure even in applications of the law of physics. In the standard theory of dyes, structural features such as the type and number of chromophores and auxochomes are considered more relevant to chemistry than magical formulas like the Schroedinger Equation and other purely formal connections to "physics".

The above considerations do not mean that chemistry is not concerned with the laws governing the behaviour of matter under the various possible conditions; but its specific laws must refer to the atoms and bonds involved in producing a given effect, rather than to the interplay of mechanical and electromagnetic principles.

The historical perspective

Thus, the whole problem of the nature of chemical explanation rests on the nature and scope of chemistry such as has been gradually shaped by history, and such as is embodied in the mentality of chemists. Now, the latter are interested in "ordinary" matter, and specifically in its composition, in the molecular and atomic constitution of its components, and in the transformations (at the microscopic as well as at the macroscopic level) of "substances" into one another. One might wonder whether this really means anything more than an artificial limitation in depth of the level of explanation. There are two ways of resolving this doubt. First of all, as has been mentioned, the attempt to replace the theory of chemistry by computations has not been received with favour by experimental chemists because it is no help in constructing a system of rules connecting structure withproperties; and therefore its does not even help in analytic and synthetic problems.

Secondly, recent progress in biology and the elaboration of system theory have convincingly shown that a complex of interdependent parts cannot be described without the introduction of categories which cannot be discovered by any amount of reflexion concerning just the parts and their interactions.

The identity crisis of chemistry is comparatively recent. To Boyle's "Sceptical chemist" not only was the search for "substances" an obvious goal of natural philosophy, but there was ground to believe that an "architectural principle" was at work in the Physical Universe. Although this notion could not imply in 1661 as much as it would have three centuries later, it certainly defined the line which eventually resulted in the modern rules of directed valency: for it placed emphasis on structure already at the dawn of molecular theory. The definitive specification of the paradigm of chemical explanation goes back, in our opinion, to Lavoisier's Traité of 1789. There the "ultimate principles" to which chemical facts should be brought back were operationally defined as the "elements", viz. those substances which chemical analysis could not further decompose. Of course, this characteristic feature is also a highly questionable point, because it assumes that chemical analysis is rigorously defined; which it is not. This difficulty, however only points to the need of taking historical aspects into account when dealing with different branches of a single body of knowledge-natural philosophy: it is only too natural that in order to draw lines of separation in such a "compact" field of knowledge one should resort to tradition.

Nevertheless, there is one way to circumvent this necessity; a which paradoxically but luckily, brings us back to reductionism. The latter is probably not a delusion, if it means that there are some unifying principles of all sciences. Indeed, in this sense physics has actually the merit of having most striven towards finding and stating those general concepts and the principles governing them. One such concept introduced even before the formal separation between physics and chemistry is energy. Now, physicists classify phenomena according to the energies required to study them experimentally. This criterion places chemistry in the electron-volt (ev) range. Thus, a reasonable definition of chemical analysis would be: decompositions of materials that can performed by using energies not greater than a few ev. This is more satisfactory than a definition merely based on tradition. In fact, even though it cannot replace the latter (because the concept of chemical analysis is needed to preserve the distinction of chemistry from disciplines like optics), it helps to place chemistry in the context of science; the more as the same energy classification can be useful in defining biology. On the other hand, both biology and chemistry require the above-mentioned concepts of "complexity level", a concept until recently extraneous to physics. Energy-range considerations do define operationally the classes of experiments reaching the various levels of complexity; but the ontological dimension must be added to it to provide an assessment of the programmes and types of explanations characteristic of different sciences.

Conclusion

The arguments given in support of the specificity of chemical explanation can be summarized by restating what we think is the emerging outlook on the unity of science. There are a few basic principles which hold for all natural sciences: the conservation of energy (possibly in its relativistic form), the second principle of thermodynamics, perhaps principles based on general symmetry laws, and perhaps others. They are the foundation of all sciences: biology, physics, chemistry, cosmology.

Then there are classes of questions. Tentatively, three examples can be given: 1- how can this phenomenon be described in terms of first principles, and the motions of the ultimate constituents of matter? (This is the request for a "physical" explanation); 2 - What entities and related structural rules are responsible for the facts observed? (This is the "chemical" explanation, and applies to nuclear physics because nuclei have a scientific status equivalent to that of molecules at the next lower level of complexity); 3- to what function does the observed behaviour of the given entity correspond? (This is just one possible form of a request for biological explanation; that control-system studies involve the same kind of questions simply means that biology has historically restricted its field to natural self-regulated systems).

If this picture is correct, what remains of the claim of physics to be the queen of the sciences? That claim, it must be emphasized, has nothing to do with the claim of some physicists that only physics is real science. In fact, the above example suggests that physics, in its proper sense of science of motion and forces, has a special programme: instead of stopping at a given level of complexity, it goes on indefinitely in a bathogenous plunge towards first principles and the ultimate constitution of matter. In this respect it is unique. But that reductionist process requires dropping all that arises when parts are combined to form wholes. This is why, in spite of that fascinating programme, other sciences have something original to contribute to our knowledge of the physical Universe.

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