Chemistry and Complementarity *

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Abstract

The molecular view haunted chemists for a long time. Since this vision promised an outline of chemical reality in terms of basic building blocks, complementary approaches were neglected. Nowadays, the molecular program of chemistry has arrived at its successful termination so that the theoreticians find themselves challenged by new ways of looking at familiar facts of chemistry.

Our modern theoretical first principles allow a precise mathematical definition of Bohr's notion of complementarity and enforce a pluralism in looking at the nature of things. In particular, complementarity is revealed with conspicuous clarity everywhere in chemistry. The complementary aspects of classical and quantal descriptions of molecules and the complementarity between molecules and chemical substances are discussed. The discourse is concluded with a hint of how chemistry could help in learning complementary ways of thinking and to place complementarity into a wider perspective.

IT IS A PURE ILLUSION TO THINK THAT LEARNING ALL ABOUT TINY THINGS IS THE PATH TO KNOWLEDGE ABOUT BIG THINGS. *C. A. Truesdell* [1]

1. On the viability of the molecular view

The breathtaking success story of the atomistic and mechanistic approach to the study of natural phenomena has profoundly affected the way scientists think. The molecular view has triumphed in physics, chemistry and biology with immense practical results. Particle physics and molecular physics explain a wide range of phenomena qualitatively and quantitatively, and in harmony with experience. In high-energy physics and in biology the fascination of atomism has not lost its power.

A large majority of physicists enthusiastically supports the latest quark models and the grand unified theories. Quarks, together with leptons and vector bosons, are regarded as the ultimate primitive objects which should form the basis of a fundamental understanding of nature. The atomic view is very much alive in present-day high-energy physics, some of its supporters even expect it to reveal the deepest mysteries of being.

In the last decades molecular structure has become a matter of primary interest to biologists. Molecular biology has produced a profound new understanding of the way cells are made and the way they work. Nowadays molecular biologists achieve miraculous things, such as the synthesis of enzymes, which were considered impossible a few decades ago. A precise knowledge of the structure of biomolecules is a must for a real understanding of many fundamental life processes. So the molecular view is full of life in contemporary biology.

As opposed to the situation in high-energy physics and biology, atomism is an old and not very exciting story in chemistry. In the main, chemistry has fulfilled its molecular program. Molecular chemistry produces new but not unanticipated knowledge. All essential details of the outcome of a new experiment are either known in advance or they can be calculated from the fundamental theory. In this sense, pure molecular chemistry starts to become boring. In fact, many science students prefer as a research topic either high-particle physics or molecular biology where they hope to find unexpected hence exciting new facts.

On the other hand, just the fact that molecular chemistry is an essentially closed field with a sound theoretical basis makes it a most interesting object for theoretical reflections. Since science is concerned with truth, not utility, the practical success of the molecular view is no proof for its veracity. Does the molecular view really tell the truth, the whole truth and nothing but the truth? Our main thesis is that the richness of chemical phenomena renders it impossible to discuss them exhaustively from a single point of view. We need many complementary views, all of them are a priori equally fundamental and merit equal theoretical status. The molecular view is just one of these views and has no privileged status. The atomic idea is a myth.

2. The atomic myth

Every civilization has its myths which the members of the group share in common. Myths are not fictions but sacred traditions which demand unqualified faith. A myth tells how something came into being, so it is always related to a "creation" [2]. This explanation may sound strange to modern scientists. Nevertheless, the contemporary atomic idea and molecular view still contain aspects of the old atomic myth.

In the 17th and 18th century the idea of indivisible particles was quite popular and the advocates of the "mechanical philosophy" accepted atomism on faith and without logical evidence. For example, *Isaac Newton*'s natural philosophy was atomistic. In his Query 23 of the Latin edition of his *Opticks* in 1707 (renumbered 31 in the second English edition of 1717) Newton defended atomism as follows: "... it seems probable to me, that God in the Beginning form'd Matter in solid, massy, hard,

* Elaboration of a lecture "Chemie und Komplementarität" delivered at the Chemische Gesellschaft Zürich in February 1982.

impenetrable Particles... even so very hard, as never to wear or to break in pieces; no ordinary Power being able to divide what God himself made one in the first Creation" [3].

Nowadays we have evidence for the existence of atoms and molecules. Many scientists even believe in the objective existence of quarks, leptons, vector bosons, atoms and molecules since they believe in the existence of unproblematic facts of nature. It is worthwhile to remember that historically the almost universal acceptance of the atomic idea as a scientific fact is related to the *theory* of Brownian motion.

When tiny particles of microscopic size are suspended in a fluid they carry out a peculiar haphazard movement that never ceases. This phenomenon was already known to the inventor of the microscope, *Antony van Leeuwenhoek* (1632–1723). He and the early investigators seem to have assumed that these particles were alive. The first serious investigation is due to the distinguished Scottish botanist *Robert Brown* (1773–1858) who in 1827 demonstrated the presence of this motion in living as well as in nonliving matter and refuted experimentally facile explanations such as convection currents or temperature-gradient effects. For a long time the true nature and the cause for this apparently spontaneous motion could not be clarified but after 1878 most scientists attributed it to thermal molecular motions. However, the majority of scientists still had not yet a true understanding of the cause of Brownian motion: it is tempting to think that the curious zigzag trajectory of a Brownian particle is due to kicks from exceptionally energetic molecules. But this is certainly not correct, each collision with a single molecule has an entirely negligible effect. The correct explanation was known to *Carbonelle* (1874) and *Delsaulx* (1877) who stressed that the Brownian motion has to be considered as a fluctuation phenomenon, due to the fluctuations in the accumulation of an enormous number of collisions.

The decisive breakthrough in the understanding of the phenomenon of Brownian motion is due to the theoretical work by *Albert Einstein* (1905) and independently by *Marian von Smoluchowsky* (1906). Both Einstein and Smoluchowsky showed that to a first approximation the coordinate of a Brownian particle as a function of time defines a sample function of a Markovian stochastic process. Einstein's and Smoluchowsky's theory of Brownian motion was finally established by the experimental work of *Jean-Baptiste Perrin* in the years 1908 and 1909. These experiments led to a determination of Avogadro's number by Einstein's diffusion equation for the probability density of the Brownian stochastic process, and therewith to a universal acceptance of the molecular and kinetic view.

A landmark in the history of chemistry was the conversion of the fanatic critic of atomism, *Wilhelm Ostwald*. In 1908, he wrote in the preface of the fourth edition of his famous text «Grundriss der allgemeinen Chemie»: «Ich habe mich überzeugt, dass wir seit kurzer Zeit in den Besitz der experimentellen Nachweise für die diskrete oder körnige Natur der Stoffe gelangt sind, welche die Atomhypothese seit Jahrhunderten, ja Jahrtausenden vergeblich gesucht hatte. ... Damit ist die bisherige atomistische Hypothese zum Range einer wissenschaftlich wohlbegründeten Theorie aufgestiegen» [4]. The conversion of Wilhelm Ostwald had a great influence on the further development of chemistry. While the molecular view fell on fertile ground, the further development of a theory of chemical substances was deprived of intellectual incentive. Even today, chemical thermodynamics and chemical kinetics are still on the rudimentary stage of development achieved at the turn of the century. The molecular idea flourished and degenerated into a dogma requiring unqualified faith.

3. Demythologization by quantum mechanics

The development of quantum mechanics led to three results of great importance for chemistry:

(i) The molecular view got a sound theoretical foundation, based on first principles.
(ii) The atomic myth was broken.
(iii) The idea of complementarity got a precise expression.

While the first result is well known among chemists, the second and the third point deserve some elaboration.

Paul Tillich calls a myth which is *understood as a myth* but which is not eliminated, a *broken myth*. The task of every demythologization is the breaking of myths, not their elimination. A broken myth represents a partial truth, not the whole truth but one aspect of the truth. It is not appropriate to characterize a broken myth in terms of truth and falsity. While a myth demands faith, a broken myth can be endorsed in terms of effectiveness and ineffectiveness. Quantum mechanics leads to a demythologization of the atomic myth by disclosing its group-theoretical background and by refraining from the ontological claim that elementary particles are ultimately real things.

In addition, quantum mechanics sheds a fresh light upon this situation by explaining why every description of nature reflects at most a *partial* truth. Nature must be seen not from one side alone but from all sides. Such complementary descriptions disclose different aspects of the same truth.

4. The end of the Cartesian-Newtonian epoch

The elementary systems as described by quantum mechanics are very different from Newton's "solid, massy, hard, impenetrable particles". An electron is neither solid, nor hard, nor impenetrable. Moreover, our theoretical viewpoint is markedly different from that of a classical scientist. We have learnt that natural laws are not really *descriptions* of nature but rather *prescriptions* to scientists to act in certain ways rather than in others. Furthermore, it has been suggested "that it would be useful to replace the idea that scientists are the passive *discoverers* of the unproblematic facts of nature with an alternative view that instead they actively *construct* their world" [5].

The classical conception is closely connected with the idea of an "isolated system". Of course, isolation from the environment is never perfect, nevertheless the concept of an "isolated system" is a useful approximation for many problems of classical science if we correct for the small interactions with the surroundings.

In quantum mechanics there exists a new type of typically quantum-mechanical correlations, the so-called *Einstein-Podolsky-Rosen correlations* leading to holistic effects which cannot be reduced to interactions of any parts of the whole.

Remark: Holistic system

It is a mathematical property of all classical theories (like Newton's mechanics, Maxwell's electrodynamics or Clausius' thermodynamics) that the state of all the subsystems of a given system determine the state of the whole system; this property is called *separability*. A system is called *holistic* if it does not possess the property of separability. That is, a holistic system cannot be decomposed into nontrivial subsystems in such a way that the states of the subsystem determine the state of the whole system. Since the state-space of quantum mechanics is not a simplex, quantum mechanics is a holistic theory. For a more detailed discussion compare [6].

If we take quantum mechanics seriously it refers to the undivided wholeness of nature. The undivided whole is patternless, absolutely no patterns are visible without breaking the holistic symmetry. In quantum mechanics there are no isolated systems unless *we* isolate them by neglecting the Einstein-Podolsky-Rosen correlations between the object and its environment. There is no such thing as a perfect description of nature: ***every testable description of nature describes only certain aspects and neglects other aspects.*** The existence of Einstein-Podolsky-Rosen correlations implies the existence of *incompatible* aspects, that is, aspects which cannot be put in evidence in one and the same description. In quantum mechanics, patterns arise by breaking the holistic symmetry, they are generated by abstracting from particular Einstein-Podolsky-Rosen correlations. Every abstraction represents a particular perspective so that complementary abstractions lead to complementary viewpoints.

It goes without saying that in its quantum-mechanical description the world appears very differently structured from what the Cartesian-Newtonian view understands by the "empirical world". *René Descartes* (1596–1650) wrote: "I have described ... the whole visible world as if it were only a machine in which there was nothing to consider but the shapes and movements" [7]. This paradigm leads to the belief in the existence of a single frame of reference for the description of reality. However, the holistic character of nature forces us to allow for incompatible viewpoints. Quantum mechanics is the first mathematically formulated holistic theory. While Descartes sharply distinguished between matter as simply extended substance ("res extensa") and mind as unextended thinking substance ("res cogitans"), in quantum mechanics there is no ultimate division between the observer and the observed object.

5. Origins of the notion of complementarity

Niels Bohr's conception of complementarity marks a singular turning point in the development of science. It was in September 1927, during the commemoration of the hundredth anniversary of Volta's death in his native city of Como, that Bohr introduced the term "complementarity" to describe the relation between classically incompatible aspects of a situation whose complete description must incorporate both aspects [8]. The incompatibility of complementary phenomena is not a logical but a dialectical contradiction. From an experimental point of view, complementary phenomena involve the same system, but manifest themselves only in experimentally incompatible situations.

While Bohr's concept of complementarity has a unique position in the history of physics, the underlying idea is as old as religious and philosophical thought. Even in physics, the complementarity of the particle and the wave description of light has historical precedents. Commenting on the controversy concerning Newton's corpuscular theory and Euler's wave theory of light, the famous *Georg Christoph Lichtenberg* (1742–1799) wrote: "Es kann bey einem so verwickelten Streite, wie der über die Theorie des Lichts, wo Newton und Euler an der Spitze der Parteyen stehen, nicht mehr schlechtweg die Frage seyn, was ist hierin wahr? Sondern, welche Erklärungsart ist die einfachste? ... Wie wäre es, wenn man am besten damit auskäme, beyde Theorien des Lichts, die Newtonische und die Eulerische, zu vereinigen?" [9].

Bohr made it very clear that the notion of complementarity is not restricted to quantum physics. He stressed that this idea is related "to the general difficulty in the formation of human ideas, inherent in the distinction between subject and object" [8].

Remark: A more recent characterization of complementarity

It is difficult to find in the works of Bohr a really satisfying characterization of the notion of complementarity. The best formulation I know is due to Klaus Michael Meyer-Abich: «Komplementarität heisst die Zusammengehörigkeit verschiedener Möglichkeiten, dasselbe Objekt als Verschiedenes zu erfahren. Komplementäre Erkenntnisse gehören zusammen, insofern sie Erkenntnis desselben Objekts sind; sie schliessen einander jedoch insofern aus, als sie nicht zugleich und für denselben Zeitpunkt erfolgen können. Die Struktur des Objekts, die darin zum Ausdruck kommt, dass es komplementär erfahren und beschrieben wird, kann mit Bohr als Individualität oder Ganzheit bezeichnet werden» [10].

After complementarity had been accepted in quantum physics, it was tempting to resolve other apparent contradictions in the description of nature in terms of complementary descriptions. Bohr himself came to believe that the idea of complementarity can be extended into areas such as biology and psychology and finally to the whole range of human intellectual experience [11–14]. For example, Bohr saw relations of complementarity between instinct and reason, individual and society, compassion and justice. Nowadays it is common jargon to call any dialectic opposites "complementary pairs". Famous examples are: conscious and unconscious [15, 16], intellectual knowledge and sensuous knowledge [17], causal description in space-time and synchronicity [18], structure and function, mechanistic biology and vitalism, biological structure and biological information [19], the rationality of science and its irrational origin, scientific knowledge and mystic knowledge. Whether all these examples do justice to Bohr's intuitive notion of complementarity is doubtful. The extension of the idea of complementarity to wider problems is dangerous and demands a deep intuitive understanding. In order to avoid vague notions, we prefer an analytical formulation which can be motivated by Bohr's writings and which can be rigorously extended to a large class of mathematically formulated scientific theories.

6. The logic of complementarity

Complementarity emerged as a fundamental trait in the discussion of quantum phenomena. The gist of quantum mechanics lies in comprising all the possible complementary descriptions within a single logically consistent theory. If the idea of complementary modes of description is to have practical import in a more general theoretical framework it has to be formulated as a logical relation between statements, that is, as a kind of nonclassical predicate calculus, called *complementarity logic*.

In the formalism of quantum mechanics, the time-honored particle-wave duality is replaced by the complementarity of position and momentum. The criterion for two physical quantities to be incompatible is the *noncommutativity* of the observables representing the two quantities. For example, in quantum mechanics the observables Q and P of position and momentum fulfill the canonical commutation relation

$$QP - PQ = i\mathrm{h}/2\pi$$

where h is Planck's constant. Two quantities are complementary if they are maximally incompatible. More precisely, we have the following definition: *two physical quantities are called complementary if there exists no state in which both corresponding observables have values within any finite interval.*

This definition can be simplified by stressing its logical purport. By virtue of the spectral theorem, every observable can be decomposed into elementary observables whose spectra consist of at most the values 1 and 0. These so-called projectors represent *propositions* about yes-no experiments indicating whether or not some event has occurred. In terms of these elementary observables we have the following simple characterization of complementary quantities: *two propositions are complementary if there exists no state such that both propositions are truth-definite* (i.e. such that they have either 1 or 0 as value). The non-commutativity of the projectors representing the corresponding propositions is a necessary but not sufficient condition for their complementarity.

Remark: The formal definition of complementary propositions
The set of all propositions of any physical theory is an orthomodular lattice. The orthocomplement F' of a proposition F is the negation of F (i.e. if F is true then F' is false, and if F is false then F' is true). The meet $F_1 \wedge F_2$ of two propositions F_1, F_2 represents the most general proposition which implies both F_1 and F_2. The trivial proposition which is always false is denoted by 0. With these logical notions we have the following definition: *Two propositions F_1 and F_2 are called complementary if they fulfill the relations*

$$F_1 \wedge F_2 = F_1 \wedge F_2' = F_1' \wedge F_2 = F_1' \wedge F_2' = 0$$

All mathematically formulated physical theories have a natural lattice structure. In classical theories (such as Newtonian mechanics) the propositions corresponding to the elementary observables form a *Boolean lattice* with a natural interpretation as a classical two-valued logic which accepts the doctrine that every proposition is either true or false (*tertium non datur*, i.e. the law of excluded middle). The logic arising from quantum mechanics gives rise to a genuine nonclassical logic, called *quantum logic* (a rather unfortunate name since quantum logic has nothing to do with Planck's quantum of action). Unlike the Boolean logic associated with classical theories, quantum logic is a nondistributive lattice. In a classical logic there exist no complementary propositions. The nondistributivity of quantum logic reflects the fact that quantum mechanics allows complementary quantities.

The aim of quantum logic is to grasp the various possible complementary view-points into a coherent unified theory. Its foundations were laid some fifty years ago and it has been developed vigorously in the last few decades (for a review, compare sect. 4.4 in [6]). However, classical logic retains its validity in the description of particular viewpoints. According to Bohr "all experience must ultimately be expressed in terms of classical concepts" [20]. In quantum theory, a particular frame of reference is given by the experimental arrangement. Even in microphysics, every experiment must be described in terms of classical physics whose propositional logic is Boolean "since the word 'experiment' can in essence only be used in referring to a situation where we can tell others what we have done and what we have learned" [21].

Classical Boolean logic is compulsory for an unambiguous communication but it is not only wrong in microphysics but in all sufficiently general domains. It is true that one can always restrict the universe of discourse in such a way that classical logic is valid. But such a restricted universe of discourse may be too small for an interesting description of natural phenomena. This restriction of the validity of classical logic is in substance the principle of complementarity. Hence we can interpret quantum logic (i.e. the formal logical structure of quantum theories) as a logic of complementarity.

7. Complementary theories

All the great physical theories which are relevant for the chemist (such as Newtonian mechanics, continuum mechanics, electrodynamics, thermodynamics, quantum mechanics) can be embedded into a *covering theory T* which is characterized by its logical structure and the intended universe of discourse.

The covering theory T is in the first place a language which provides us with the vocabulary to express the most diverse problems in a unified way. The proper choice of the covering theory depends on the universe of discourse. We may select it as the smallest theory containing all known relevant theories for the chosen universe of discourse. The covering theory is neither a mechanics nor a theory with any specific physical content but it represents the undivided wholeness of the universe of discourse. This wholeness is broken by a particular viewpoint represented by a *subtheory*, say T_α, of the covering theory T. Each subtheory is characterized by the abstraction leading to the particular viewpoint, and inherits the tacit prepossessions and the logical structure from the covering theory.

Remark: Algebraic structure of the covering theory
Since all known chemically relevant physical theories have an orthomodular logic, the covering theory is supposed to possess an orthomodular propositional calculus. Experience with quantum mechanics (which is not a covering theory but nevertheless has some traits of it) suggests to choose as logic the projection lattice of a factorial W^*-algebra of type I_∞. The examples we give below are based on this choice but the general discussion is independent of it.

Clearly, quantum mechanics has to be a subtheory of the covering theory of all chemically relevant theories, so that the covering theory T contains complementary propositions. This fact implies that the family of all subtheories of T cannot be totally ordered [22]. We say that T_β is a subtheory of T_α if the lattice of propositions of T_β is a sublattice of the lattice of propositions of T_α. In this case we write $T_\alpha \leq T_\beta$ and say that the theory T_β can be deduced from T_α (or also, that T_β can be reduced to T_α). The relation $\leq$ defines a partial ordering in the family of all subtheories. If the covering theory is not classical, this partial ordering is not total, that is, there exist incomparable subtheories. In analogy to the definition of complementary propositions as maximally incompatible propositions, we define *complementary theories* as subtheories of one and the same covering theory which are maximally incomparable.

Remark: The formal definition of complementary theories
Let $T_\alpha \leq T$ and $T_\beta \leq T$ be two subtheories of the covering theory T. The theory $T_\alpha \wedge T_\beta$ is defined as the largest theory which can be deduced from T_α as well as from T_β, $T_\alpha \wedge T_\beta \leq T_\alpha$, $T_\alpha \wedge T_\beta \leq T_\beta$. Furthermore, $T_\alpha \vee T_\beta$ is defined as the smallest theory from which both T_α and T_β can be deduced, $T_\alpha \leq T_\alpha \vee T_\beta$, $T_\beta \leq T_\alpha \vee T_\beta$. The complementing theory T_α' of a theory T_α is defined by the relations $T_\alpha \wedge T_\alpha' = T_o$, $T_\alpha \vee T_\alpha' = T$, where $T_o = T'$ is the trivial theory. With this notion, we adopt the following definition: Two subtheories T_α, T_β of a covering theory T are called complementary if they fulfill the relations.

$$T_\alpha \wedge T_\beta = T_\alpha \wedge T_\beta' = T_\alpha' \wedge T_\beta = T_\alpha' \wedge T_\beta' = T_0$$

For more details, compare sect. 5.5 in [6].

This digression into formal theoretical considerations may have been forbidding for non-theoreticians. It was necessary to show complementarity is neither a vague notion nor does it encourage the dark tendencies of irrationalism as claimed by some critics.

8. The complementarity of classical and quantum mechanics

Quantum logic is prior to mechanics. Mechanical systems are defined within the framework of quantum logic by the appropriate kinematical group which has to be represented by the symmetries of quantum logic. The kinematical group refers to our space-time concepts, for chemical problems it is given by the *Galilei group*. A system which preserves its individuality under Galilei transformations is called a *Galilei system*. If a Galilei system cannot be decomposed into two or more Galilei systems, it is called an *elementary Galilei system*. Mathematically speaking, elementary Galilei systems are ergodic representations of the Galilei group by the symmetries of quantum logic.

According to the representation theory of the Galilei group, the elementary Galilei systems are characterized by a triple (m, s, h), where m is a real number, $2s+1$ a natural number, and h a nonnegative number. If we put $h=0$ and $s=0$, we recover *classical mechanics* with Newton's point particles of mass m as elementary systems. If we choose h to be Planck's constant, m the mass of the electron, and $s = ½$, we recover *quantum mechanics* with electrons of spin ½ as elementary Galilei systems.

This discussion reveals that if we choose quantum logic as the basic theroretical language and if our viewpoint singles out the space-time behavoir and the atomic idea, then we recover two historically well-known theories: classical point mechanics and quantum mechanics.

The smallest covering theory for classical point mechanics and quantum mechanics which leads to a continuous dependence on the parameter h is the so-called standard representation of a factor of type I_∞. In this standard representation quantum mechanics and classical point mechanics are embedded as *complementary theories*.

This fact is of great importance for molecular chemistry. We can describe molecular systems by quantum mechanics. The description is correct and convenient for the discussion of high-resolution spectroscopic experiments. However, these purely quantal molecular systems are *not* the molecules of the chemist since they have no structure characterized by a structural formula. For example: the quantum mechanical ground state of NH_3 is *not* pyramidal with the nitrogen nucleus at the vertex and the three hydrogen nuclei forming the base. This classical feature arises only in a mixed quantum-mechanical/classical description which in contemporary quantum chemistry is generated by the so-called Born-Oppenheimer "approximation". However, this chemically relevant description is by no means an approximation, it is complementary to the purely quantal description. Neither description is more correct than the other, neither can replace the other, neither can be subsumed into the other, both are correct and indispensable for a complete description of the molecular reality. The domains of validity of these two complementary descriptions are subject to reciprocal limitations which prevent any logical contradiction.

9. The complementarity of substances and molecules

Contemporary chemistry tends to treat chemical substances as broken up into molecules which are considered to exist in their own right. In some cases this molecular view does not work very well. For example, liquid water is supposed to be a pure chemical substance but to this day nobody has been able to advance a sound *molecular* argument in support of this claim.

Remark: What are chemically pure substances?
Purity is the most fundamental concept of chemistry. This notion is badly neglected in modern introductory texts, presumably because the authors are mistaken in their opinion that the notion of chemical purity can be reduced to molecular concepts. That a molecular definition of pure chemical substances is not feasible is discussed at great length in the outstanding "Lehrbuch der Thermostatik" by *van der Waals* [23] (what a pleasant surprise to see a textbook the title of which clearly shows that the authors know what they are writing about). The crucial practical criteria of chemical purity (such as boiling point, freezing curve, phase rule) are of thermodynamic nature so that it is very unsatisfactory that the texts on thermodynamics have to assume that we already know what chemically pure substances are. At present this circular reasoning cannot be avoided. The theory of chemical substances is in an intolerable state of affairs.

After more than a 100 years of research in statistical mechanics and over 50 years of intensive efforts in quantum mechanics, we still do not yet understand why there are just *three* states of aggregation. We have some ideas how to describe the solid and the gaseous state but we do not yet know how to characterize a liquid in terms of molecular interactions and correlations. There are some vague ideas but in the main we are put off until later.
Supporters of the molecular view are not discouraged by the practical failure to reduce chemical phenomena to molecular interactions. Failures can always be accounted for by the inadequate state of the present knowledge. It is indeed impressive how many experts have the absolute faith that, say, the behavior of liquid water will be reduced to interacting H_2O molecules some time in the future.

Remark: Two quotations
In volume 1 of the comprehensive treatise on water, edited by Felix Franks, the molecular dogma is stated by *C. W. Kern* and *M. Karplus* as follows: "Since quantum mechanics provides an accurate description of molecular phenomena, a detailed understanding of the water molecule is available from theory. This implies that it is possible, in principle, to predict the structure and properties of water ..." [24]. In volume 6 on "Recent Advances", W. G. Richards says: "Calculation based on a brute force approach have not contributed anything of outstanding significance, while even more thoughtful attempts to use ab initio calculations as the lead to more approximate treatments still seem promising rather than definitive" [25].

It must be emphasized that the issue which concerns us here is *not* the question of accepting one theory as true and rejecting another as false. According to a time-honored cliché the criterion of truth is the verification by experiment. However, experimental data can be interpreted in more than one way. We have to investigate carefully how much or how little of our theoretical knowledge goes into the analysis of experiments. In addition to the molecular view there are conceptually different viewpoints which should be cultivated in order that the molecular idea does not end as a not-to-be-questioned dogma which cannot be modified, extended or discarded as a result of further research. Only by investigating other approaches it comes to light in what the molecular view closes its eyes to.

Example: the theory of chemical kinetics is in a bad shape
The attempts to reduce the age-old phenomenological laws of chemical kinetics to molecular collision theory led to a marked conceptual stagnation in chemical kinetics. For example, to describe enzyme kinetics in analogy to molecular-beam kinetics has no rational basis but rather belongs to science fiction.
Presently we hardly have the rudiments of a theoretical kinetics of chemical substances. The principal reason is that the interest in a genuine theory of chemical substances was overshadowed by the success of the seemingly more attractive molecular program.

Our vision of the world will be severely limited if we restrict ourselves to the molecular view. Molecular theories describe *some aspects* of matter correctly but it is not wise to think that they give us a description of reality "as it is". If we approach matter from a molecular point of view we will get molecular answers and our molecular theories will be confirmed. But different viewpoints are feasible. Questions of a different kind can be asked, nature will then respond in a new language.
A widespread category mistake in chemistry is the confusion of thermodynamics with statistical mechanics, of chemical kinetics with collision theory, and taking the concept of chemical substances as being on equal footing with molecules. Substances are either gaseous, liquid or solid – molecules are not. Substances have a temperature, molecules do not.
The molecular view does by no means follow from quantum theory. Quantum logic allows other frames of reference. One of the most interesting results in modern algebraic quantum theory is the classification of descriptions of nature according to the type of the algebras of observables. In his fundamental work on operator algebras, *John von Neumann* (1903–1957) classified the so-called W*-algebras into three main types I, II and III. The historically well-known particle descriptions in classical and quantum mechanics result in algebras of type I. In their quantum-logical interpretation the algebras of type II and III lead to completely new possibilities in the mathematical description of nature.

Nowadays we know that thermodynamic systems have an algebra of observables of type III. Since the notions of temperature and chemical substances are intertwined, we can state an important result of modern algebraic quantum theory in the following form: *molecules are described by quantum theories of type I while chemical substances are described by theories of type III.* These two descriptions refer to different planes of the same reality, they are mutually exclusive but nevertheless both indispensable for chemistry.

Remark: Niels Bohr's Faraday lecture
It was pointed out by Niels Bohr in his Faraday lecture in 1930 [26] that the description of macroscopic systems in terms of the dynamics of molecular motions is complementary to the thermodynamic description. The conditions allowing a complete mechanical description exclude the possibility of applying thermodynamic concepts. On the other hand, to assign a definite temperature to a system requires conditions of observation under which the particle dynamics escape control.

The molecular theories of type I are well-developed, what we urgently need in chemistry are competing research programs, for example a fully developed type III theory of thermodynamic matter. The development of a truly modern chemical thermodynamics and chemical kinetics as type III theories would allow a much simpler description of macroscopic matter than it is possible from the molecular viewpoint, and would lead to a fruitful synthesis of dialectic opposites.

Remark: The gauge group generates both molecular and substantial chemistry
The symmetry breaking which leads to different molecular species is the socalled *gauge group*. The gauge group for n species is the n-dimensional torus group. Different molecular species are distinguished by *classical* observables which in quantum mechanics are generated by the action of the gauge group in an algebra of type I.

The gauge group is also responsible for the emergence of different chemical potentials characterizing the different chemical substances in quantum theories of type III (such as chemical thermodynamics).
In the same way as the Galilei group generates two complementary mechanical theories – Newtonian mechanics of mass points and quantum mechanics of electrons – the gauge group generates two complementary versions of the notion of species – different kinds of molecules and different kinds of substances. Newtonian point particles and electrons are very different objects but have analogous features because both are elementary realizations of the Galilei group. In a similar fashion molecules and chemical substances have a common group theoretical background but nevertheless they are not related in a simple manner.

10. Wider implications of complementarity

By asserting its complete independence of other forms of learning, modern scientific thought has lost its last link to philosophy and humanities. Fortunately, there are strong tendencies in contemporary culture favoring complementary modes of orientation. In this situation, chemistry is in the unique position of offering an opportunity to recognize the wisdom of complementary views and to learn complementary ways of thinking by means of simple and well-understood examples.
In quantum mechanics and in theoretical chemistry we accept the necessity of complementary viewpoints. None of them is more authentic than the others, none can replace the others, all are necessary, none is sufficient. The truth about matter is to be found only by admitting all possible frames of reference. Every concept of natural science is relative to the observational means which defines the appropriate frame of reference. Every experimental fact is conditional and context-dependent. The quantum logical fusion of complementary frames of reference creates aspects which did not exist before and allows us to see the universe of discourse as a unified whole.
If we want to explore nature, we have to choose an appropriate context. *Invention is prior to discovery:* only if we have invented a context, we can discover. Science starts with ideas, not with facts. Discoverers have a fixed point of view while inventors create new contexts. For example, Newton's remark that apples are attracted by the earth was not a new empirical fact but a great idea. New ideas are viable if they lead to new viewpoints which can be used to discover new facts.
When complementary views come togehter they may blend into new thoughts. The result is far more than a mere compromise of the various viewpoints but a richer science which stresses the holistic character of modern scientific thought. The horizon of a creative scientist cannot be stretched far enough, nevertheless science is only one of the many ways to describe some aspects of our world and it cannot define reality. While biology will continue to progress on the mechanistic road for some time, the more developed sciences such as physics and chemistry do away with the subject-object dichotomy and are nowadays more open to admit that science cannot make any categorial statements about the ultimate reality. Science, art, religion and moral philosophy do neither conflict nor have they to say nothing to each other, they rather represent complementary aspects of the same reality. All of them can be accepted, all are necessary, none of them is sufficient. Every view creates a world of possible experience and brings something new into being.

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