

## DOCUMENTS

### Rein Vihalemm: ‘On the “Two-Layeredness” of Structure and the Relation of Quantum Mechanics and Chemistry’<sup>1</sup>

Translation by Ave Mets

The new categories of Marxist dialectics—structure and elements—are particularly important for solving the philosophical questions of natural science, and, in turn, a generalisation of given natural scientific knowledge helps to elaborate on these categories in greater detail. Since chemistry is a science about specific, relatively autonomous structures<sup>2</sup> of a single matter, this “mutual interest” of chemistry and the philosophical categories of ‘structure’ and ‘elements’ is perfectly natural. A summary of the studies on the works dedicated to the inquiry of the dialectics of ‘elements’ and ‘structure’ remains outside the scope of this article.<sup>3</sup> It is, though, necessary to note that the term ‘structure’ has several meanings. In the indicated article by I. S. Alekseev, this term is considered in four different meanings: (1) ‘structure as a whole’ (the concrete interrelation between concrete parts comprised in a concrete whole), (2) ‘structure in general’ (we only know that a given object has a structure), (3) ‘all structure’ (all parts without specifying the whole), (4) ‘structure as such’ (only the connection of parts).

Since the pair of categories ‘structure’ and ‘elements’ is tightly bound to two other pairs of categories (although by no means identical to them)—to form and substance, and to whole and parts—it seems that in the general philosophical theory of the categories of elements and structure, it is necessary, in a sense, to synthesise the dialectics of substance and form, whole and parts.

<sup>1</sup> Original: Vihalemm, R. (1965), ‘O “dvusoinosti” struktury i o sootnoshenii kvantovoi mekhaniki i khimii,’ *Tartu Riikliku Ülikooli toimetised / Uchenye zapiski Tartuskogo Gosudarstvennogo Universiteta. Trudy po filosofii* VIII, vihik/vypusk 165, pp. 72–88.

Editorial note: Due to the political circumstances of the Soviet Union, authors were obliged to refer to Marxist classics in their writings. Those references are retained in this translation for historical accuracy.

<sup>2</sup> On the qualitative diversity of chemical particles see, for instance, Garkovenko, 1963.

<sup>3</sup> The relevant works are: (I) Sviderskii, 1962; (II) Sviderskii, 1959; (III) Sviderskii, 1960, pp. 70–79; Zel’kina, 1959; (I) Egorov, 1961; (II) Egorov, 1962; (III) Egorov, 1963; Valt, 1963a; Alekseev, 1963; Makarov, 1963, pp. 87–94.

Aside from that, the notions ‘structure’ and ‘elements’ occur in numerous works which are not specifically dedicated to discussing these categories.

A far more strictly and distinctly developed dialectics of the categories of elements and structure can be found in the indicated monograph by Professor V. I. Sviderskii and the thesis by A. A. Egorov, although chiefly by analogy with the dialectics of substance and form. Prof. Sviderskii (Egorov shares his views) conceives structure in only one meaning—as a principle, a system, a law of relations of elements (the developed determination of structure, according to Alekseev, is ‘structure as such’).

It seems that, next to this important line of reasoning, an analysis of the notion of structure from a different angle is of special interest, namely, when this notion comprises not only the *law of bonding* of elements, but also *availability* of those elements, compartmentalisation of the phaenomenon.

In this case, the notion of structure is, notoriously, analogous with the notion of the whole: the whole presumes the presence of parts, and structure presumes the presence of elements. Structure is generally considered not merely a concretisation of form, but also a concretisation of the whole; a specific “synthesis” of form and the whole, as it were, but also of quality and quantity (the dialectic relation between elements and structure comprises, to a certain degree, both the interrelation of parts and the whole, as well as substance and form).

What we mean by the expression ‘elements of structure’ is the *interconnected* parts of a whole. Such a more general notion of structure is meant in the discourse about the *principle of structuredness*, about the structuredness of matter, about the hierarchy of structures, etc. In this paper, we consider structure in this general meaning.

Let us attempt to consider, on the example of chemistry, the “two-layeredness” which in our opinion exists in the structure, and discuss some philosophical problems related to the structure of molecules from this perspective, especially the problem of the relation between quantum mechanics and chemistry.<sup>4</sup>

Already from the general philosophical point of view, all bodies, phaenomena, etc. are in general relatively stable state of moving matter, that is, processes. Professor Sviderskii writes in his monograph: “Insofar as each phaenomenon is relatively stable by its inherent substance, preserving its state of motion, then elements are, generally speaking, primarily continuing *processes* of different qualities” (Sviderskii, 1962, p. 13). Friedrich Engels wrote in the *Dialectics of*

<sup>4</sup> The most important work on the relations between natural sciences is Kedrov, 1962. In view of the problems inspected here, see pp. 65–74, 100–109, 54–212, 212–232, 256–257, 275–314, 314–335.

*Nature*: “The whole of nature accessible to us forms a system, an interconnected totality of bodies [...]. In the fact that these bodies are interconnected is already included that they react on one another, and it is precisely this mutual reaction that constitutes motion.” (Engels, 1939[1883], ch. III)

All matter is a constellation of processes, the “world is not to be comprehended as a complex of readymade *things*, but as a complex of *processes*” (Engels, 1946[1886], Part 4). Considering any process of this constellation, one can see that it exists by virtue of an interrelation of more elementary processes, i.e., it has a structure. Those elementary processes are the structural elements of the structure under examination.

Take the molecule of hydrogen, for instance. Classical theory asserts that it consists of two monovalent atoms, bound by a chemical bond. Why is hydrogen monovalent? Why does valence exist? What is a chemical bond? The classical theory is unable to answer those questions. Butlerov could only “anticipate” that in the future, this will be explained by “the motion of (in the chemical sense—R. V.) its tiniest particles” (Butlerov, 1953, p. 372). But in his time, no such motion was yet known. At that period, one could discern a molecule from the general constellation of processes, one could see that the molecule as a process exists by virtue of the interrelation of atoms, that is, it has a structure. But this structure (process) could only be examined down to an atom. Atom was not considered a process back then (when Butlerov inaugurated the theory of chemical structure, it was still called an atomic hypothesis!), i.e. it was not possible to *derive* molecular structure from a connection of *processes*. Interatomic relations in a molecule were only investigated based on the generalisations of given chemical reactions, and as a result, properties of atoms and interatomic relations (valences of atoms, types of relations, etc.) were uncovered. However, as long as the structure of atom remained unknown, it was in principle impossible to explain, for instance, why hydrogen is monovalent (it was not even necessary to *absolutely* confidently ascertain that hydrogen is always and in all circumstances monovalent, as this was a conclusion factually obtained from an incomplete induction), and to explain a chemical bond otherwise than simply to declare that it is “chemical”<sup>5</sup> because, even though properties, as is known, “occur in relations, and are not created by those relations, hence the definite ground of any properties must lie in the things themselves” (Sviderskii, 1962, p. 266). If only one process is investigated (in our case, the molecule, i.e., the process of atomic interrelations), while ignoring others, then it is clear that only empirical

<sup>5</sup> It was impossible to find a material carrier of chemical relations, uncover the “related elements” (see Egorov, 1963, pp. 7–8).

conclusions can be drawn from this process—‘thus, it is’. But if we deal with a process whose essence is known, then, in principle, it is also possible to determine the *essence* of that process which constitutes the interrelation of ordinary processes (in case we succeed in finding a relation between the essences, i.e., a law). But according to the law of the transformation of quantity into quality, this essence can appear as *entirely* unintelligible if we are ignorant of the “field we stumbled upon”, since we simply know virtually nothing about the new process as a whole. We know not which properties it features, since we know not which relations it enters (we know not the *phaenomena*, *essence* of which we came across!). A chemist has difficulty telling something intelligible about a multiatomic molecule when they are preoccupied with estimating the stable configuration of its nuclei and electrons, although the outcomes of this estimation indeed belong in chemistry. In general, considering the cognition of the structuredness of matter in depth, one may argue that the so-called chemical structure of molecules (the structure of atoms is not paid attention to) is only an “upper layer”, the essence of which lies deeper—in the interaction of nuclei and electrons. Niels Bohr wrote: “it is interesting to note that fruitful application of the structural formulae in chemistry rests solely on the fact that the atomic nuclei are so much heavier than the electrons” (Bohr, 1958, p. 99). Ia. K. Syrkin adds: “The great mass of nuclei enables to localise them with a high precision. But this does not apply to electrons which are smeared over all energy levels, in the general case enveloping all nuclei” (Syrkin, 1962, p. 405).

The quantum mechanical approach to the molecule of hydrogen (Heitler & London, 1927), which became the groundwork for applying quantum mechanics in chemistry—quantum chemistry—leads to all empirical conclusions. According to the Heitler-London method, two nuclei and two electrons are premised on the system. Because of the great difference in the masses of nuclei and electrons, the equations of the motion of electrons is envisaged in the force field of the nuclei.<sup>6</sup> Apparently, the covalent bond forms when the electron spins are antiparallel. This corresponds to the case when the electron shells of atoms partly overlap, whence between the nuclei, contraction of charge between electrons occurs, which also supports positively charged nuclei. Hydrogen is monovalent because it only has one electron. Helium, for instance, cannot form covalent bonds because its two electrons with antiparallel spins are already paired with each other, etc. A quantum mechanical analysis of molecules showed that all forces of chemical bonds are electrical (more precisely, electromagnetic) in nature.

<sup>6</sup> See, for instance, Veselov, 1962, pp. 96ff. For an exact solution of the quantum mechanical problem for hydrogen see, for instance, Moelwyn-Hughes, 1957, pp. 157–181.

For some reason, A. D. Vislobokov writes in his book that

the very nature of chemical bond is and remains chemical [this claim is simply tautological—R. V.]. When some physicists and chemists assert that quantum mechanics established the electrical nature of the chemical bond, then they essentially claim nothing less than that, according to Coulomb's law, a chemical bond of atoms is every time accompanied by the attraction of particles with opposite electric charges, and a chemical dissociation of atoms is accompanied by a repulsion of particles with similar charges. Neither theoretical nor factual base is available for going beyond such assertions to claim that a chemical bond only reduces to electric charge. The reduction of chemical bond to an electric and quantum mechanical one bespeaks an extreme overestimation of electric and quantum mechanical coupling in chemical bonds, the reduction of the latter to one of the subordinate couplings bespeaks a misconception that the chemical bond has its specificity and its cognition does not reduce to a cognition by physical methods. This, finally, implies exit from further cognition of chemical bond. (Vislobokov, 1962, pp. 46–47)

Yet, already in 1952, Academician A. N. Nesmeianov noted that attempts to find the “chemical force” resemble the quest for “life force” in biology. He wrote: “The molecule is, of course, a definite form built by nucleic-electric formation, and no special forces other than those known in the physics of nucleic-electric interactions prevail in its formation” (Nesmeianov, 1952, p. 198). V. A. Shtoff (1956, p. 77) and N. T. Abramova (1962, p. 55) wrote the same.

It should be noted that Engels's term ‘subordinate’

must in no terms be taken to mean ‘non-existing’, ‘secondary’. No, it (the word ‘subordinate’—R. V.) only means that a simpler form (motion—R. V.), when operating inside of a more complex one, must not be understood similarly as it is when operating by itself, outside of this more complex form [...] as the principal one. (Kedrov, 1962, p. 293, see also p. 172)

Let us consider the problem of the relation between a ‘subordinate’ and a higher form of motion, and the specificity of the chemical form of motion from the perspective of the categories ‘structure’ and ‘element’. Thereby one must primarily pay attention to the distinction of the categories ‘elements’ and ‘part’. Elements are separate constituting components of a complex subject matter or process, taken in their concrete interrelation. We speak of parts as isolated separated (or

not yet unified) elements (Valt, 1963a, pp. 45–46; see also Egorov, 1963, p. 6). If we consider, for instance, a hydrogen molecule, then it is only in a quantitative sense possible to say that it consists of parts—of two atoms of hydrogen. In the structure of a hydrogen molecule, there are no hydrogen atoms in the sense of ‘parts’, they are *structural elements*. An isolated hydrogen atom (i.e., when it is a ‘part’) has a spherically symmetric electron shell around its nucleus, no external forces affect the nucleus, etc. In a hydrogen molecule, however, it is not the case (although it does not undergo qualitative change in the sense that the chemical element hydrogen would turn into another chemical element).<sup>7</sup> That is, quantity is converted into quality: out of two hydrogen atoms, a new quality has formed—a hydrogen molecule. The whole is not a sum of parts (if not the mere *number* of parts is meant). Parts turned into structural elements. Thence it is clear that laws applicable to an isolated atom are not applicable to bound atoms. If a branch of science (in our case, quantum mechanics), by whose methods the laws of an isolated atom were obtained, were preoccupied with such a form of motion which only holds in an isolated atom, then surely it would be impossible to investigate bound atoms, i.e., molecules, by the methods of this compartment of science.<sup>8</sup> But, as is known, quantum mechanics investigates all systems with wave and corpuscular properties and discrete energy, hence also systems consisting of nuclei and electrons.<sup>9</sup> “Quantum mechanics basically has the potential to correctly explain all phenomena occurring in the electron shells of all systems, no matter the number of atoms entering the system, and therefore it is a theory both of physical as well as chemical *elementary phenomena* (my italics—R. V.)” (Veselov, 1962, p. 213). Quantum mechanical computation of

<sup>7</sup> One must pay attention to, in our view, the not entirely strict formulation by Prof. Sviderskii, which has also been supported by Egorov (1963, p. 15) that the emergence of a new structure can also be related to a new way of unification of old elements, their redeployment (see Sviderskii, 1962, p. 61; 1960, p. 76). Isomers n-butane and isobutane are given as examples. This contradicts Sviderskii’s position: “The very law of conversion of quantitative changes into qualitative ones characterises the dependence of the reconstruction of the structure of a phenomenon on the change of its elements” (Sviderskii, 1960, p. 77). The contradiction emanates from not discerning the concepts ‘element’ and ‘part’. Different structures cannot have identical elements (those structures can only be identical in *substance* that has its place in isomerism). When a new structure emerges, it does not already have ‘old elements’, they are already converted into new elements of the new structure. If we take strictly into account also the interaction between elements not immediately coupled, then we can say that isobutane has not one structural element of n-butane. How, then, can we simply talk about rearrangement of old elements (one can only restructure parts!)? (In this respect, see also the paper by Borisov, 1961.)

<sup>8</sup> On “markers” of mechanicism, see Kedrov, 1962, p. 204.

<sup>9</sup> Quantum mechanics is a compartment of science about abstract-general form of the motion of matter, but quantum chemistry is already in a seamless connection with a certain aspect of matter. In this regard, see also Kedrov, 1962, pp. 69–73, 256, 278, 282 and Solopov, 1963.

the structure of a molecule is one of the specific tasks of quantum mechanics (from which quantum chemistry emerges), the outcomes of this computation, however, belong in chemistry. The theory developed by physicists—quantum mechanics—is simply applied in a given case to compute molecular structure. Here it is appropriate to repeat the words once expressed by B. N. Menshutkin: “A physicist conceives the theory and methods of investigation, builds necessary apparatuses. A chemist’s task is to apply the readymade apparatuses, elaborated research methodology, laws deduced by the physicist, for his specific work [...] Truly chemical are only inferences from experiments.” (Menshutkin, 1937, p. 314, in this regard see also Kedrov, 1962, pp. 65–69)

As we already noted, the “pre-electric” chemistry could make only empirical generalisations about molecular structure. Molecule related to the field of chemistry only “down to the level of atom”. It was impossible to consider atom as a process; chemistry only acknowledged the properties of atoms and thereby drew conclusions about molecular structure. After the discovery of atomic structure and the emergence of quantum mechanics, it became possible to consider atoms as processes and molecules as interconnection of these processes. However, from the perspective of quantum mechanics (or more precisely, quantum chemistry), a molecule is a very complex process, since from this perspective, the properties of atoms in the structure of a molecule are unknown, but it is necessary to yield the molecular structure as an interconnection of nuclei and electrons. Quantum chemistry studies the molecule, in a sense, “on one level deeper”. Both sciences (chemistry and quantum chemistry) enable us, in principle, to determine molecular structure. Both sciences have their strengths and weaknesses, and in actual practice, develop conjointly. The unremarkable role of quantum mechanics in chemistry thus far is explained by the complexity of the mathematical apparatus, but the development of computing machines and novel computational tricks will allow to overcome those difficulties in the future. In our opinion, there is no grounds to assert (as some philosophers and chemists do) that quantum mechanics lends no help in cognising the molecular *structure*. After all, it has been shown that no specifically chemical forces exist in nature, that the interatomic bond in a molecule, which is the chemical bond, is explained by electromagnetic forces which can be calculated by means of quantum mechanics.<sup>10</sup>

<sup>10</sup> It is appropriate to mention that already A. M. Butlerov predicted this, see his 1953a, pp. 372–373, 283; 1953b, pp. 45, 75.

The specificity of a chemical bond does not emanate from some special chemical forces, but from our dealing not simply with general electromagnetic forces but with specific interatomic electromagnetic forces in a molecule which can only be detected and calculated by means of quantum mechanics. To claim that the nature of chemical bond is “only chemical” is to absolutise the specificity of chemical bond, to fetishise chemistry, to think dogmatically and simply to “forbid” cognising the *essence* of this particular bond.

Examples can be given of separate compartments of science studying one and the same object and in the end obtaining one and the same outcome<sup>11</sup> (which is entirely natural when adequate outcomes are obtained) (see Kedrov, 1962, pp. 100–103). For instance, the laws of thermodynamics can be deduced by the methods of statistical mechanics. In the relation between thermodynamics and statistical mechanics, there is much that is analogous to chemical and quantum mechanical inquiries of molecular *structure*. As is known, thermodynamics is grounded on experimental laws (the principles of thermodynamics), and one can say that, like chemistry, it is on the level of a “surface layer”. Statistical mechanics, however, derives those principles from the essence of thermodynamic quantities, it is in a sense “one level deeper”, from where it ascends “upwards” with its deductions.<sup>12</sup> Because statistical mechanics emanates from essences (more correctly, from the essence, for instance, of the second order, since the laws and concepts of thermodynamics are, after all, also the essence of some sort of order, but we have in mind the essence of the “upper layer”), its path, just as that of quantum mechanics, is considerably more complex, but at least it answers the question “why?”.

A doubt may arise: are we not overstating the role of quantum mechanics, and does it not ensue therefrom that we can regard any “higher structure” as an interrelation between nuclei and electrons. If we take a closer look at the issue, there is no risk of that.

<sup>11</sup> “One and the same outcome” must certainly not be understood in a way that the study of the object by separate compartments of science gives nothing new; it is only emphasised here that the objective ground of knowledge does not “vanish” anywhere, that the outcomes obtained by different methods of inquiry describe that object to different depths, that the results, in the end, correspond to each other but are not identical.

<sup>12</sup> For instance, statistical mechanics revealed the statistical nature of the concept of entropy (the capability of energy to transform) and showed that the second principle of thermodynamics—the law of increase of entropy—is a probabilistic law and denotes the transition of the system from less probable states towards more probable ones.



As we saw above, elements of a process generally also appear to be processes, but in the chemical inquiry of molecular structure, the elements of structure are not regarded as processes. Therefore, according to the general concept of structure, “included” in the structure of molecule are nuclei and electrons. Factually, they are also factored into the chemical account of molecular structure, since they *determine* the properties of atoms, circumscribe (although in a “withdrawn” form for a chemist) the chemical bond, etc., i.e., those ‘elements’ by which molecules find the structure. We may draw a general conclusion that the structure of a process is determined when its elements are known: (1) as processes, i.e., also the structure of the elements is known, (2) as unstructured but, in a sense, “carved-out” pieces of the structure under consideration. In the second case, we know how the structure is constituted by the elements (we learn this as a result of a generalisation from an examination of properties of this structure and of “unstructured” elements), although its essence is unknown.<sup>13</sup> In the first case, therefore, one can say that the elements of the elementary processes of a process, in a sense, also remain the elements of the process—the structure remains “two-layered”. The molecular structure can be determined by the so called chemical bond of its atoms, or the bond of the nucleus and electrons. Therefore, considering the *structure*<sup>14</sup> of molecules on the level of nuclei and electrons is fully justified. Thereby, the objective fact that “in the hierarchy of structures, their mutual influence quickly declines, and manifests itself in a decisive moment only in the framework of one order” (Valt, 1963a, p. 48) becomes important. Thus it is no longer justified to regard the structures whose elements are molecules (for instance macromolecules, chemical reaction) merely as a bond of nuclei and electrons. In the case of a macromolecule (it constitutes a new quality, a new level in the structural hierarchy, and it is dealt with by a new compartment of chemistry)<sup>15</sup>, nuclei and electrons remain on an all too “deep a layer”, although even the elementary components are connected by ordinary covalent bonds whose essence certainly remains on the level of nuclei and electrons. However, should we calculate the entire structure of a macromolecule on this level, we would not gain information about the *macromolecule*, but simply of a molecule. We could not tell the link between the structures of ‘elementary components’

<sup>13</sup> The “connecting elements”, material carriers of the connection between elements, are unknown (see Egorov, 1963, pp. 7–8).

<sup>14</sup> Let us remind ourselves that ‘structure’ does not directly equal the quality of the subject.

<sup>15</sup> See, for instance, Strepikheev & Derevitskaia, 1961; see also about the emergence of this new quality Zhdanov, 1960, pp. 179ff.

from the link between the structure of atoms (nuclei and electrons)<sup>16</sup>. While by determining the molecular structure based on the “nether layer”, the system of atoms is considered on the level of their structure (nuclei and electrons), this is done leaning on quantum mechanics, then by determining the structure of a macromolecule from the “nether layer”, it is necessary to lean on the structure of the molecule (by polymerisation—on monomers). Thereby it is crucial to consider the system of those structures in mutual influence which is emphasised by laws of chemistry, “ordinary” molecules, where the quantum mechanical laws already exist in a “withdrawn” manner.

It is further important to notice that, while considering the relations of quantum mechanics and chemistry, we only spoke about the possibility of conceiving the *molecular structure* by quantum mechanics. After all, the main object of chemistry is structure, where the inner molecular structure changes (often an intermolecular process, but generally some sort of interaction of molecules with the surrounding medium), i.e., a chemical reaction which can be viewed as an instance of intensive structure.<sup>17</sup> Taking into account the above-indicated conclusion about the possibilities to determine the structure, for a chemist it is important, first of all, to know molecular properties which manifest in this intensive structure. (Chemists do study those properties experimentally, too.) But since properties depend on the nature of the subject, a chemist also needs to know this nature, determine the quality of the subject as structure (Madiarody, 1962), i.e., one must consider also the “nether layer” of the structure of a chemical reaction, whose elements are chemical atoms. Thereby the research object of chemistry consists in the unity of interatomic extensive and intensive structure.<sup>18</sup> Chemistry pays attention to the inquiry of such unitary structure, i.e., the dependence of reactivity of molecules on their structure is inquired. The question arises whether one should not consider the elementary act of such a unitary structure quantum-mechanically.

M. G. Veselov writes:

A pertinent task in contemporary quantum chemistry is the elaboration of quantum dynamics of elementary chemical processes. The theory of

<sup>16</sup> The structural hierarchy studied by chemical sciences (that is why they are sciences) can be further specified, discerning inorganic and organic molecules, molecules of complex compounds, etc.

<sup>17</sup> On the concepts intensive (process) and extensive (subject) structure, see Sviderskii, 1962, pp. 19–20.

<sup>18</sup> Tracing such unitary structures is one of the aims of the analysis of extensive and intensive structures (see Sviderskii, 1962, p. 120).

stationary molecular states merely allows to obtain some backhanded answers to partial questions touching upon the field of chemical reactions and reactivities. Creation of a theory of *elementary chemical act* (italics by me—R. V.) appears to be a fairly difficult task and, at present, its solution is unclear. We can only say that this task consists in elaborating a theory of collisions of atoms and molecules in very complex circumstances. (Veselov, 1962, p. 212)

Here the task is set perfectly correctly—a new structure requires a new theory. If such a theory will be elaborated, then apparently it will be the core of the chemical theory. (Since the core of the *chemical theory* cannot be *chemical*: chemistry remains on the “upper layer”, while physics is on the “nether layer”.) The results obtained with the help of this theory will, however, belong in chemistry and acquire its new qualitative substance *on the basis of chemistry*.

Is not this mechanism? We believe that this is the same kind of ‘mechanicism’ as deriving the laws of thermodynamics with the help of statistical mechanics. While thermodynamics only studies one process, statistical mechanics opens the core of that process taking into account elementary processes, examining them in their interactions, it arrives at a new quality that the separate elementary processes do not possess. We also showed that this is possible with respect to the concept of structure.

As is known, a new quality arises as a consequence of quantitative changes in an old quality. A new structure (process) arises as a consequence of a coupling of more elementary structures (elementary processes). Reduction of a new quality to an old one, of a new structure to an old one (of a process to elementary processes) takes place when we, in the sphere of the new structure, new quality, attempt to stay on the level of the old structure, old quality, without taking into account the changes which they undergo. In this case we would be dealing with an explicit mechanism, and we can be convinced that such inquiries do not yield the desired results. A new quality, a new structure must be considered not merely “in a ready state”, as it were, but also from the perspective of the old quality, of the elementary structures on the new level, that is, the old structure together with the quantitative changes (= already the “embryo” of the new quality), elementary structures in their interrelations (= already as the “nether” layer of the new structure). This seems to be the only way if one wants to clarify the rise of a new quality,<sup>19</sup> and to go from the level

<sup>19</sup> On genetic approach, see Kedrov, 1962, pp. 169–175; 193–197.

of ‘thus, it is’ to the level ‘why thus is’, ‘where does this arise from’. But such an approach is significantly more complicated, since structural elements, and consequently their interrelations, are extremely abundant. After all, as already noted, one cannot simply complicate the results obtained from a problem of *isolated* elementary structures, but instead their interrelation needs to be found, i.e., an entirely new problem has to be solved—to address the structure on the level of the elements of its elementary structure (here one certainly has to take into account what has been said in fn. 7).

Often structures are first considered “in a ready state”, qualitatively, since their specificity appears earlier, and only later attempts are made to also *deduce* this structure from a “nether layer”. “Human thought goes endlessly deeper from appearance to essence, from essence of the first order, as it were, to essence of the second order, and so on to no end.” (Lenin, 1976[1915])

Let us now try to detail the meaning of “two-layeredness” of structure and, along with this, the relation of quantum mechanics and chemistry, keeping in mind the circumstance that the

quantum mechanical facet sticks out, in the case of higher forms of motion, merely as ‘auxiliary’, not at all as principal. It unavoidably has to be recognised, otherwise addressing the corresponding higher forms of motion is not possible either in the genetic or in the structural profile, meaning that the higher form of motion itself remains unexplained in its essence. (Kedrov, 1962, p. 305)

However, the quantum mechanical regularities “manifest their undeniable and huge cognitive import only in the cases, with rare exceptions, when the question is about construing, from a physical perspective, regularities which have previously been found by chemistry” (Kedrov, 1962, p. 319).

We showed above that by establishing the “upper layer” of the structure, structural elements are known because their properties are generalised, i.e., regularity is established by studying the qualitative facet of a phenomenon. By establishing the “nether layer” of the structure, however, structural elements are known as processes, as elementary structures, i.e., there are known regularities, and one has to find a new regularity, but already theoretically, moving to ideal-concrete (see also Zhdanov, 1963, pp. 51–57), to the side of the ‘more complex reality’ (than the one from which one departed). Thereby no idea of its qualitative facet is held, even though the bases of all properties are known

(true, those properties are only potentially possessed) (Kedrov, 1962, p. 179).<sup>20</sup>

Kedrov depicts the relation of atomic-electronic physics and chemistry as follows:

chemistry  $[A] \rightarrow M$

atomic-electronic physics  $[e^-, N] \rightarrow A$

(M—molecule; A—atom; N—atomic nucleus;  $e^-$ —electron. In square brackets—the initial “cellule”, for the given science, see Kedrov, 1962, p. 228)

To depict the relation of those sciences with the recognition of *molecular structure*, we get:

chemistry  $[A] \rightarrow M$  (“upper layer”)

atomic-electronic physics  $[e^-, N] \rightarrow M$  (“nether layer”)

Since the subject of atomic-electronic physics is the motion of electrons in the force field of a nucleus, but molecules do not form *immediately* from nuclei and electrons (see Kedrov, 1962, pp. 321–325) in chemical processes,<sup>21</sup> then the possibility of reducing chemistry to physics always *remains* a mere *possibility*. As soon as we start realising this possibility, we no longer stay in the sphere of physics, but proceed to a science about a relatively higher structure of matter—chemistry. This structural level is governed by its own objective laws which express the qualitative facet of this level which is inaccessible to the laws of a lower structure, which can only explain this level from a quantitative aspect (see Kedrov, 1962, p. 334; in this connection see also Kivenko, 1960, pp. 158–164). *Both sciences have different cognitive resources and must consider themselves in consonance.*

That is indeed how they appear, whereby *model concepts* serve as “mediating stations” (see Valt, 1963b, and literature included there, see also Shtoff, 1963). In fact, in all quantum mechanical computational methods of molecular

<sup>20</sup> Inter alia, the possibilities of exposed regularities are in general considerably broader than this reality in which they are exposed, but all those possibilities must still find a way to be realised. Exactly this, for example, is the task of the so-called technical sciences (the problem of establishing the ‘second objective reality’). Besides, some theoretical sciences deduce laws whose meaning is until now entirely unclear, as long as they do not get “help” “from the other side”, via the qualitative facet of the phenomena (for instance, a majority of mathematical theories).

<sup>21</sup> Besides, we always underlined that, by addressing the relations between quantum mechanics and chemistry, we only mean elementary chemical phenomena. For real chemical processes, see, for instance, Kedrov, 1962, pp. 325–326.

structure<sup>22</sup>, model concepts are applied, since the mathematical complications of quantum mechanical computations require finding simplified methods.<sup>23</sup> Application of models allows regarding the structure just barely “a layer deeper”, rather somewhere “in the middle”. For building those models, high quality data from chemical theory are extremely important as well.

Observable and unexplainable, as Bykov (1959, p. 516) writes, the coincidence of results obtained in computations performed on the basis of different models is explained from the perspective of “invariance” of theory with respect to the model upon which it is built (Valt, 1960, p. 101; 1963b, p. 15).

Comparing the listed computational methods (see Bykov, 1959, p. 516), it turns out that the method of molecular orbitals appears to be the closest to the real situation, and, in this light, it is also the most complicated of all. Since in the method of molecular orbitals, the motion of each electron is considered in the force field of the nuclei and the rest of the electrons, the structure is deduced from the “nether layer”; interatomic interactions and the fact that all electrons participate in forming a bond are taken into account right from the start. But if we are “located” on the “upper layer”, then we have to discern different types of bonds (ionic, covalent, hydrogen, coordinate bond and others) which emerge as a result of interatomic interactions.

For example, the compound of ammonia and trimethylboron cannot be explained either by an ionic bond (neutral molecules) or by a covalent bond (no unpaired electrons). Such a bond is called a coordinate. A compound with such a bond (complex compounds) is often encountered in inorganic chemistry.<sup>24</sup> The founder of those theories was the German chemist A. Werner (1893). Relying on empirical material, he came to the conclusion that next to the so-called primary valency there is also a so-called secondary valency. Werner also introduced the notion of coordination number which remains one of the main concepts of complex compounds. Secondary valency is encountered in the case of ammonia and trimethylboron, too. Werner wrote:

<sup>22</sup> For instance, the theory of directed valency, which evolved from the Heitler-London method; the valence-scheme superposition method; method of molecular orbitals; electron gas model, including many varieties, among which the most important is the free electron model, and others. A review of those methods can be found in Bykov, 1963; Veselov, 1962; Shtoff, 1963, pp. 74–126.

<sup>23</sup> This appears to be a habitual strategem in many cases with concrete tasks of quantum mechanics (see Valt, 1960, p. 105).

<sup>24</sup> Few are such bonds in organic chemistry since carbon is a unique element in the periodic system (see, for instance, Syrkin, 1962, p. 401).

The secondary valencies chain with one another, by atomic bonds, radicals which cannot form stable bonds with their own kin, so, for instance in  $(\text{H}_3\text{C})_3\text{B}\dots\text{NH}_3$  radicals  $\text{B}(\text{CH}_3)_3$  and  $\text{NH}_3$  are chained by a boron nitride bond, while neither  $(\text{CH}_3)_3\text{B}-\text{B}(\text{CH}_3)_3$  nor  $\text{H}_3\text{N}-\text{NH}_3$  exist. (Werner, 1902, p. 273 cited in Bykov, 1960, p. 232)

This is a very characteristic conclusion which can be drawn on the basis of the factors of the “upper layer”. It is, again, another ‘thus, it is’ statement, but at the same time a very important one, since a new property of atoms in molecular structure is exposed. In the “nether layer” there is no need and no possibility<sup>25</sup> to discern between different types of bonds, since chemical bond rises as a result of the electron “smearing”. When explicating the perspective of the method of molecular orbitals, Syrkin draws attention to compounds for the description of which the existing concepts are not sufficient (for instance, that a bond only forms on the expense of valence electrons, etc.) (Syrkin, 1962, p. 405).

Let us make a few additional general remarks related to the “two-layeredness” of structure.

Engels, underlining the unity of discreteness and continuity, wrote: “The new atomistics is distinguished from all previous to it by the fact that it does not maintain (idiots excepted) that matter is *merely* discrete, but that the discrete parts at various stages [...] are various *nodal points* which determine the various *qualitative* modes of existence of matter in general” (Engels, 1939[1883], Section ‘Notes and fragments’). Zhdanov writes:

It is important to emphasise that the structural-dynamical levels of organisation of matter possess a relative independence and closure. Exactly because of this it is possible to study them relatively independently from each other, occasionally carrying out inquiry on the higher level without yet having a full conception of the mechanisms on the lower one. (Zhdanov, 1961, p. 17)

We have shown that, by studying *only* the higher level, it is not possible to thoroughly understand the essence of the phenomena under investigation and to learn how they arise. One always gets to the point where one cannot say more than: this is what practice tells us for now. If new “disruptive” facts emerge, one must look for new, more general laws, but one never has a solid

<sup>25</sup> However, in this, in fact, also manifests the restrictedness of quantum mechanics in chemistry, its so-to-say non-sensibility and incapacity of qualitative conclusions.

guarantee that “nothing more will happen” (this were only possible with a plain induction). It appears appropriate to note that, in view of the objective existence of relatively independent structures of matter and their hierarchy, new sciences and disciplines have emerged and still emerge. Thereby three kinds of sciences or disciplines can be discerned among them. Firstly, sciences which deal with one concrete structure on the level of its “upper layer” (for example, chemical sciences). Secondly, sciences which study a concrete structure on the level of its “nether layer”, discovering the *essences of the laws* of the “upper layer”, explaining empirical laws theoretically (which means that the laws of the “upper layer” obtain another foundation and do not require a full induction of empirical facts). Among such sciences, for instance, is quantum chemistry.

One might ask whether we are equipped to sufficiently “trust” the laws about the “lower” structure (since the theory of the “upper” structure leans on those laws on the level of its “nether layer”) by explaining the laws of the “upper layer” of the “higher” structure? Certainly one has to bear in mind that the “lower” science must itself be sufficiently developed, understanding of the “upper layer” of its material structure must in general be completed before this “lower science” can help the “higher” one. Cognition, however, evolves from the essence of the “first order” to the essence of the “second order”, etc. and that which for the “nether layer” remains the essence of the “first order” will, for the “upper layer”, be the essence of a deeper order. Further movement of the “lower” science to the essence of a deeper order has no considerable impact on the “upper” structure, since the essence of the first order remains the “upper layer” of the material structure of the “nether” science under investigation and the “nether layer” reached in further cognisation remains too deep for the upper structure due to an immediate interaction between different structures only in the limits of one order (i.e., recognition of the structure as only “two-layered” is justified). Since in nature (especially in living nature), too, such complex structures exist whose elements on one level are different “lower” structures, then studying them on the level of the “lower layer” requires a synthesis of various concrete sciences (for example, molecular biology).

Finally, and thirdly, abstract sciences which investigate certain abstractly discerned facets from one, few, or even all concrete material structures, regarding also interstructural transitions (for example, mechanics, mathematics, cybernetics, the general systems theory of L. Bertalanffy and others). Thereby a no unimportant part is played by the fact that in the structural hierarchy of matter, structures of different orders and their mutual relations are generally



analogous. This circumstance lies at the heart of abstract-general sciences which encompass the general features of all material structures (to this also relates, inter alia, materialist dialectics as the most general science). The theories and methods developed by those abstract sciences are, on their part, applied by concrete sciences (the sciences of the first and second kind) to investigate the separate facets of concrete structures.

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