The Epistemological Status of Theoretical Models of Molecular Structure

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Abstract: For many decades, chemists regarded rigid models of molecular structure as representing structures of real molecules as their attributes. However, new experimental data required a new theoretical conceptualization. The rigid model has been replaced with a dynamic model in which molecular structure is changed under the influence of environmental conditions. The above case shows some problems connected with recognizing theoretical models as structural representations of real empirical systems. Owing to the fact that theoretical models of molecular structure obtain local interpretations with a procedural character, they can be carriers of specific information about structures of real molecules. Finally, I argue that, although theoretical models can be well corroborated empirically, they cannot be treated as representations of real empirical systems but can play a very important role in experimental practice.

Keywords: *rigid and dynamic model of molecular structure*, *representation*, *quantum theory of molecular structure*, *local interpretation with procedural character*.

Introduction

The theoretical research practice of chemistry consists to a considerable extent in constructing theoretical models without which experimental practice would be impossible. The most widely known theoretical models of chemistry are those of molecular structures of chemical compounds. According to the fundamental paradigm of chemistry, chemical structure is regarded as an intrinsic and unchangeable molecular property. It is assumed that it would be impossible to explain and predict the course of chemical reactions without the knowledge of it. However, in contemporary theoretical chemistry the assumption that the structure of the molecule is its attribute is increasingly being questioned. Modern, very precise methods of experimental determination of molecular shape make chemists-theoreticians replace the rigid model of

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molecular structure with its dynamic model. In the present paper, I will be defending the position according to which the passage from the rigid to the dynamic model of molecular structure is connected with the change of its cognitive status. Rigid models have generally been regarded realistically as it was assumed that they represent the structure of real molecules. From the point of view of the dynamic model, the molecular structure depends on experimental and measurement circumstances. For this reason, the instrumentalist-pragmatic interpretation seems to be more justified.

I suggest explaining that fundamental cognitive difference by referring to the distinction between structural and informational models. Rigid models of chemical structure have been seen as structural models as it was assumed that they represent the structure of real molecules. In the first part of my paper, I am trying to justify the belief that the theoretical model cannot be referred directly to the real object being modeled, but only to its theoretically conceptualized form. Analyzing problems connected with a referential and procedural interpretation of the language of the theory in which the model in question is being constructed, I am trying to demonstrate that in a number of cases the theoretical model can only be seen as an informational model. The informational model of the empirical system provides information about it but does not remain in the relation of similarity with its structure. In Section 3, I suggest seeing dynamic models of molecular structure precisely as informational models. I regard the above position as moderately antirealist. From its perspective, it is no point in talking about structure as an intrinsic, unchangeable molecular property. All bits of information provided by the dynamic model of molecular structure depend on the energetic state of the molecule and measurement techniques applied.

1. General methodological considerations about empirical systems and their theoretical models

We will consider the concept of 'theoretical model x' as a theoretical model of an empirical system that can be both an empirical object and a range of possible empirical phenomena as well. Theoretical models may be built for particular individual empirical systems, as well as for types of these systems. Empirical systems investigated in science are not given directly, although when we are dealing with macroscopic objects we may cherish such an illusion. Empirical systems occur in science in a theoretically conceptualized form which means that sets of measurement points and sets of magnitudes determining their characteristics are provided.[1] Sequences of dimensional values of these magnitudes, obtained from measurements, are subsequently cor-

related with appropriate elements of theoretical models and form the basis for the determination of empirical adequacy or the degree of empirical confirmation of the latter. Conceptualizations that constitute empirical systems (objects of scientific investigation) are of a theoretical nature, and that is especially obvious when we consider systems that are not directly observable. The same object of investigation can be conceptualized intentionally in a number of ways. Its particular conceptualizations can differ from one another in theories on the basis of which they are made, in the choice of sets of measurement points as well as in quantities that constitute a given conceptualization.

Considering theoretical models of particular empirical systems, we distinguish them from semantic models of theories on the basis of which the former have been built. The application of semantic models was associated with the program of logical reconstruction of scientific knowledge, for it was precisely for empirical theories reconstructed on the basis of logic that methods worked out within model-theory semantics were used. They made it possible to explicate many concepts useful for the analysis of scientific knowledge and to answer a number of important questions in methodology of empirical sciences. However, the application of model-theory methods was connected with the acceptance of numerous and strongly idealizing assumptions which have brought about the questioning of the usefulness of the concept of semantic model for the investigation of empirical knowledge for a long time.[2] What was first of all stressed was the fact that it does not correspond to the intuitions representatives of empirical sciences associate with the concept of model. In order to render these intuitions a concept of theoretical model was suggested whose content and extent were determined in a large number of ways. For the purposes of the present paper, it is convenient to make use only of a general concept of theoretical models. Such a concept leaves room for supplementing results from detailed analyses of theoretical models constructed in science and it plays well the role of an instrument to analyze various functions performed by these models in research practice of empirical sciences.

The characterization of the theoretical model that meets the above requirements was formulated by P. Achinstein.[3] It consists of five postulates providing features that distinguish precisely enough a class of theoretical models both from other types of models and from scientific theories. Achinstein's proposal can be easily applied to investigate particular models constructed in empirical sciences and supplemented by results of analyses of detailed aspects of these models.

Achinstein's account of theoretical model is a set of assumptions and postulates that refer to any empirical system. These are general conditions determining the way of solving a given research problem, formulated in some

language that is usually mathematized and interpreted. In the conception of theoretical models presented here, the particular problem and the degree of adequacy with which it should be solved is regarded as their constitutive feature.[4] The second feature of theoretical models is that they are constructed in order to show the inherent structure, composition, and mechanism of the object (system) being modeled. Another feature of theoretical models is that constitutive assumptions are seen as approximations useful for certain research purposes. What is also essential is that they are constructed on the basis of theories that are more fundamental. Thus, when we say about a theoretical model that it is a theory, then it is a theory of a given object or phenomenon, or objects or phenomena of a certain type. However, as we shall demonstrate in the next Section, the theoretical model is generally given a different interpretation than the theory in the conceptual apparatus of which it was built. The determination of relations between the theory and the theoretical model is further complicated by the fact that it is often constructed on the basis of several different fundamental theories which can be incompatible with one another. What is also important in distinguishing between theoretical models and theories is the fact that theoretical models need not necessarily be fully deduced from the theory in question but can also be supplemented by other assumptions such as *e.g.* empirical generalizations, hypotheses *etc.* The fifth feature of theoretical models identified by Achinstein is that they can bear resemblance between the object or system being modeled and other empirical objects or systems.

Quantum mechanical models describing the distribution of charge density in a molecule are examples of theoretical models constructed in chemistry. They could be regarded as equivalents of classical models of chemical bonds. The most widely known theories of quantum chemistry on the basis of which these models are constructed are the theory of valence bonds and the theory of molecular orbitals. These theories have been formulated within the framework of quantum mechanics and can be regarded as different methods of solving the approximate Schrödinger equation for electrons in molecules. Models constructed in a conceptual apparatus of these theories meet fundamental postulates formulated by Achinstein.

The above presented characterization of theoretical models allows the same empirical object (or system) to be modeled by many possible models, depending on the problem we are supposed to solve with the help of them, on the adequacy of its solution, and on theories on the basis of which these models are constructed. In addition, it has to be stressed that we always build theoretical models for empirical systems which have been conceptualized previously.[5] The choice of conceptualization depends on the conceptual apparatus available in which we can describe a given object. For a researcher, to provide a conceptualization is to constitute an object being modeled as an

object of scientific research; *e.g.*, the conceptualization of molecular shape consists in the choice and definitions of parameters that will determine it (for more details, see Sect. 3). That point becomes especially evident when objects being modeled are from the micro-world. Only after a certain conceptualization of these objects, the semantic relations determining the correlation between elements of the model and elements of the theoretically conceptualized empirical system being modeled are possible.

The above function of interpretation makes it possible to translate sentences about the model into sentences about the theoretically conceptualized empirical system; thus, it is a semantic function. It differs from the semantic function providing referential interpretations for the empirical theory on the basis of which the theoretical model was built. The referential interpretation of the language of an empirical theory is a universal interpretation that is not unambiguous. The universal interpretation determines the denotation of fundamental terms of the empirical theory and determines the class of its semantic models. In formal methodology of empirical sciences, it is demonstrated that it is impossible to determine a single proper (intended) model of a given theory. However, an unambiguous referential interpretation of the language of the empirical theory does not determine the ambiguity of the interpretation of theoretical models built in a conceptual apparatus of this theory. For theoretical models may possess an unambiguous local interpretation determined by means of proper measurement procedures. Theoretical models are built "in order to experimentally test specific hypotheses. They provide interpretations of the terms of the theory [in which models are built, P.Z.] by justifying experimental procedures for testing hypotheses stated in those terms. The interpretation of this kind might be called procedural."[6] The procedures in question provide terms of the theoretical model with unambiguous interpretations which makes it possible to formulate sentences whose logical values are subsequently determined empirically. Let us note, though, that it is only the previous conceptualization of the empirical object (system) that enables us to identify particular empirical data (measurement results) as representing particular features of this object (system) and, consequently, to use these data for testing the theoretical model. As we shall show by taking models of molecular structures as an example, the situation described above is even more complicated when we are building theoretical models for objects from the micro-world. For these models provide solutions to problems put forward in values from the micro-level, while values obtained from measurements are from the macro-level.

The outlined problems associated with the reference of theoretical models to the empirical objects (systems) being modeled makes us take precautions when trying to characterize the representational function ascribed to theoretical models. Precautions are even more recommended because the theoretical

conception on the basis of which the conceptualization of a given empirical object (system) is made does not have to be the same as the one to which we refer when building its model.

In constructing theoretical models in research practice of empirical sciences, a very important role is played by the methods of experimental research. The application of particular experimental and measurement techniques as well as their accuracy have often an influence on the shape of our research problems for which we build the theoretical models. The development of new methods may cease earlier constructed theoretical models performing the function of useful research instruments. Problems may also appear in the course of referring experimental data to the model. Data obtained with the help of various measurement procedures may be interpreted in different manners which may make it impossible to refer them in an unambiguous way to quantities that occur in the model.

2. The controversy about the cognitive status of theoretical models

Theoretical models of empirical objects and phenomena perform various functions in science. One of the most fundamental of them is representing, which has been explicitly expressed in Achinstein's definition. However, in the context that is of interest to us here the term 'representation' (and 'to represent') is at least ambiguous. It can be used in such a sense in which we are saying that a picture by a realistic painter presents (represents) the landscape painted by him or her or in such a sense in which a lawyer represents his or her client in court.[7] These two senses are constantly confused with each other. There is an important difference between them. The representation in the first sense assumes a structural similarity between objects that are representing and those that are represented. In the second sense of the term in question it is assumed that the object that represents is merely a vehicle of some information pertaining to the object represented and therefore it cannot play the role of its image.

I shall name theoretical models that represent in the first sense of the term 'structural models' and theoretical models that represent in the second sense of the term 'informational models'. Structural models are characterized by similarity to empirical systems being modeled. What I have in mind here is similarity with respect to selected features and relations. The relation of similarity is homomorphism, and in extreme cases, it is isomorphism. The informational model of the empirical system is a model that provides information about the system but does not remain in the relation of similarity with re-

spect to its structure. Obviously, a structural model is at the same time an informational one, but not the other way round.

Arguments in favor of seeing theoretical models as informational models come from the problems connected with referring the theoretical model to the empirical system being modeled. I have dealt with these problems in Sect. 1. The information (data) about the system as a result of measurements depends on the way of theoretical conceptualization of the system studied and the measurement procedure and it changes together with the change of circumstances. As a consequence, the similarity relation between the model and the real system cannot be determined. We also encounter additional problems if the system being modeled is an object from the micro-world. It has to be remembered that the information about the object being modeled provided by the informational model is relative to the above mentioned factors. Therefore, some philosophers of science deny that informational models have any cognitive value. In Sect. 3, I aim at demonstrating that the dynamic model of molecular structure can be regarded only as an informational model, as opposed to the rigid model that have been regarded as a structural model.

Some contemporary philosophers and sociologists of science have seriously questioned the possibility that the various 'products' of scientific research can perform the function of representing at all. With respect to theoretical models, the traditional controversy was between supporters of the realistic interpretation and supporters of the constructivistic interpretation of their cognitive status. In contemporary philosophy of science, the creative (constructive) character of the process of theoretical modeling in empirical sciences is usually not questioned any more. However, from that does not yet follow the ascription of an instrumental function to theoretical models. Whether holding a realistic or an antirealistic version of constructivism depends to a large extent on the way the very issue of representation is explicated. An example of a realistic kind of constructivism in philosophy of science is provided by the position of R. Giere. The author rejects extreme realism according to which the relation of structural similarity between the model and the object being modeled holds with respect to all its known features and relations. Due to the aspectual character of theoretical models, similarity relations may hold only in certain respects and to a certain degree.[8]

Thus, Giere regards a theoretical model as an 'insufficient' representation of the empirical system – as a construct which is a symbolic and at the same time a simplified representation of the object being modeled, *i.e.* a structural model that retains only some features and relations of the empirical system. The relativization introduced by Giere obviously does not help to overcome problems connected with the construction of the similarity relation, problems which make many philosophers of science refuse the realistic status of theoretical models. B.C. van Fraassen, a recent advocate of constructive em-

piricism, takes precautions against it and claims that it is impossible to state in a legitimate manner a similarity relation between parts of the model and non-observable features and relations of the system being modeled.[9] Similarity may only occur between an empirical substructure of the model and observable aspects of the system being modeled. A theoretical model as a whole can only be empirically adequate. In B.C. van Fraassen's view, his position is supported by the occurrence of empirically equivalent theories which differ in ontological postulates as well as by different applications of the principle of minimization of assumptions to ontological and epistemological problems. For similar reasons, van Fraassen's position is regarded as modestly antirealistic.

Philosophers of science who doubt that theoretical models can perform the function of representing in the first sense of the term are followers of a different sort of constructivism. They believe that theoretical models can be merely informational models rather than structural ones. They are first of all followers of constructivism in sociology of science – a current that is inherently differentiated. Representatives of the so-called strong program of sociology of knowledge believe that theoretical models are products of scientists as means to predict, plan, and control future events.[10] All these actions are possible because they refer to the real world, although models cannot represent it in a structural sense of the term. If they are to perform the above functions, it is sufficient that they are informational models that serve as useful instruments to intervene in nature. We are right now referring to the distinction introduced by I. Hacking – a leading representative of the 'new experimentalism' – between representing and intervening.[11] The use of structural models for representing makes them perform, beyond others, cognitive functions in science. Informational models, on the other hand, perform utilitarian functions first of all.

A still more radical position is taken by followers of the so-called macroconstructivism in sociology of knowledge: B. Latour and S. Woolgar.[12] They cancel the distinction between the external world and the model. Any preference for a certain kind of interpretation is not based on its cognitive value, nor on its pragmatic features that would depend on the system being represented, but arises from the social competition between groups of scientists who are trying to impose their ways of representing on each other.

The fundamental argument put forward by opponents of the traditional, *i.e.* structural, view of representing is that it is impossible to accept a transcendent point of view from which one could determine the relation between the model and the object being modeled. The latter always has to be expressed in some language. Thus, one could ask, "What do theoretical models constructed by scientists refer to?" The analysis of research practice of empirical sciences shows that, although scientists intentionally construct models

for real empirical systems, as a matter of fact they always refer to their theoretically conceptualized forms. If the theoretical model cannot be directly referred to particular empirical systems, then it is impossible to determine its adequacy with respect to its extent.

As we have already said, referring the model to the empirical system is always made owing to a theoretical conceptualization of the latter. The above conclusion expresses one of 'methodological horrors' of representation stated by macro-constructivists. It is the mutual dependence between the representation and the object represented.[13] On the one hand, the object represented determines features of the representation and, on the other hand, the representation determines features of the object represented. Thus the components of the pair: representation/the object represented cannot be analyzed separately because they are mutually dependent on each other.

The model, or actually the theory, based on which it is constructed enables the conceptualization of the empirical system. Values of magnitudes obtained from measurements have empirical sense and can be the basis for the verification of values obtained from the model only if they are interpreted on the basis of an appropriate empirical theory. Empirical values have procedural interpretations as they are determined by methods of their measurement, and these are always of theoretical nature. Theoretically interpreted results of measurements can in turn influence the modification of existing models or the construction of new ones. Let us note that usually there are several methods to determine the value of a given physical magnitude and in some cases they can refer to different theories. Thus, as another of 'methodological horrors' of representation distinguished by Woolgar,[14] representing is always of an inconclusive character. Each representation refers to a different representation and is explained by it. The theoretical model refers directly to a conceptualized empirical system; thereby it refers to a certain representation of experimental data rather than to a real empirical system.

Contrary to realists, I will thus claim that there is no function that enables direct translation of sentences about the model into sentences about the real empirical system. However, the theoretical conceptualization of the system being modeled enables to correlate values of magnitudes of the model and values of proper magnitudes obtained from measurements. Therefore, the theoretical model is able to provide information about the object being modeled. The following question has to be answered, though: why do we recognize as illegitimate the inference of the structure of the real empirical object from the structure of the model of its conceptualized form? Thereby we come to still another 'methodological horror' of representation. Representation can indicate an empirical system; but it cannot depict it, for it can determine neither isomorphism nor homomorphism between the model and the system, owing, for instance, to a selected set of features and relations. In

science, one often builds models of the same empirical system based on different, sometimes incommensurable, theories. If these models are structurally different but empirically equivalent, then it is impossible to make a choice between them on empirical grounds and decide which model represents the structure of the real empirical system. Therefore, what seems to be justified is the position that regards theoretical models as informational ones. An exemplification of the above consideration will now be the analysis of theoretical models of molecular structures of chemical compounds.

3. From a rigid model to a dynamic model of molecular structure

It is assumed that the molecular structure of a chemical compound is determined by three elements: constitution, configuration, and conformation. Constitution means a certain manner and sequence of bonding of atoms. Configuration is defined by a spatial arrangement of atoms, which is in turn characterized by valence angles of all atoms that are directly linked to at least two other atoms. Finally, conformations of a given molecule are different, thermodynamically stable, spatial arrangements of its atoms resulting from rotations around single bonds.[15] However, for the determination of the molecular structure working chemists usually provide the following three parameters: distances between atoms, angles between bonds, and their directions, *i.e.* gradients of electronic density. The two former parameters determine the symmetry of the molecular shape, while the third determines its electrical and magnetic properties.[16]

The commonly accepted and, more importantly, commonly used model of molecular structure has been a rigid or semi-rigid one. The model has been constituted on the grounds of three theories: Butlerow's, Kekulé's, and van't Hoff's theory of molecular structure; Lewis' electronic theory of chemical bonds; and the theory of molecular wave mechanics. However, the representation of molecular shape of chemical compounds was already possible on the grounds of Butlerow' and Kekulé's theory of molecular structure itself, started in the middle of the nineteenth century and then developed by van't Hoff. According to the latter, the theory of structure of chemical compounds deals with the spatial position of particular atoms with respect to one another in a molecule, without taking into consideration the character of forces that bind them.[17] Thus, this theory had a merely geometrical character. That was overcome only when Lewis' theory of electronic bonds was formulated. The two theories were the core of classical structure theory according to which structure is an attribute of a molecule of a chemical compound. Owing to the ac-

ceptance of several idealizing assumptions, classical structure theory could be subject to formalization and axiomatization and then rules of generating models for particular molecules could be determined.[18] These models were abstract structures fulfilling axioms of the theory discussed, and thereby could be recognized as its semantic models. Thus, the rules generated were in fact the rules providing a universal semantic interpretation for terms of classical structure theory.

However, these rules did not determine in an unambiguous way the class of semantic models for this theory and made it even possible to construct models devoid of an empirical sense. Only models that possess a geometrical representation have empirical sense. The rules of empirical representation were introduced with the help of A. Tarski's geometry.[19] Owing to them models of molecular shape of particular compounds were obtained that possessed procedural interpretations determined by methods of experimental determination of molecular shape. These models had also visual representations called Stuart models. However, classical structure theory did not generate satisfying models for aromatic compounds such as benzene. There were attempts to solve the problem by ascribing several structures to a single aromatic compound. The resonance theory was one of these attempts, and resonance structures of aromatic compounds were treated in a purely instrumental way.[20]

It was necessary to reformulate some elements of the classical model in the conceptual framework of quantum mechanics. As a result, there appeared a model based on several fundamental theoretical postulates. It was assumed that molecular electronic states can be separated from their rotational and vibrational states. All energetic changes associated with the three kinds of energetic states in this model are approximately independent from one another and can be considered separately. Of crucial importance for the molecular shape in this model is the fact that rotational and vibrational spectra can be measured separately. Thereby, the molecular shape (bond lengths and angles, vibrations performed) is constant and approximately independent of the degree of rotational or vibrational excitation.[21] Molecular electronic states in this model are calculated by means of a time-independent Schrödinger equation for an individual molecule. In this account, electrons are described in a quantum mechanical way, while nuclei are treated in a quasi-classical way. In 'classical' molecular quantum mechanics, a molecular structure is defined via the Born-Oppenheimer potential surface. One can use 'classical' quantum mechanics as a starting point, and derive molecular structure as an asymptotic 'concept' in the singular limit of infinite molecular mass. In quantum chemistry, the two most widely known approximation methods for solving the electronic equation are the molecular orbital and the valence bond approach. However, "the Born-Oppenheimer approximation is usually satisfactory for

ground electronic states of neutral molecules; its failure in the excited states of polyatomic molecules and ions is a common occurence".[22]

The above-presented 'classical' quantum theoretical model of molecular structure can be tested by means of experimental methods. Spectroscopic methods play a particularly important role. It has to be mentioned, though, that quantities whose values are obtained from spectroscopic measurements are macroscopic quantities (*e.g.* distances between spectral lines) and they serve to determine microscopic magnitudes (*e.g.* distances between atoms). What holds while determining the latter quantities is Heisenberg's uncertainty principle which make it impossible to determine precisely *e.g.* both the location and the momentum simultaneously. This principle does not hold while determining values of macroscopic magnitudes. The above example demonstrates that procedural interpretation of theoretical models can be complex and can encounter interpretation problems as "data from the space in which Heisenberg's principle does not hold are used to obtain information about the space in which it holds".[23] These problems become serious when results from macro-scale measurements are combined with values obtained from a theoretical model. Depending on the experimental method applied, we obtain different definitions of distances between atoms. For example, it is possible to determine a so-called equilibrium distance between atoms of a given molecule by means of microwave spectra. The distance between atoms is then assumed to be the distance between their nuclei, as calculated from the rotational spectra. On the other hand, electron diffraction data may be used to calculate the distance between atoms, defined now as the mean value of the distances between centers of the electronic clouds of atoms.[24] Thus, an unambiguous referential interpretation of the term 'distance between atoms' is not possible. Only local interpretations of that term have an empirical sense. Their procedural character is related to a particular method of measurement. "Hence, there is probably no wonder that, even for small molecules, it is been found that different experimental methods may lead to different molecular structures, indicating that no such unique structure exists."[25] The molecular shape determined by a model depends on the applied measuring procedure as "each experimental method introduces its own transformation of data from the micro-space to the macro-space".[26]

In the process of constructing theoretical models, the precision of measuring methods by means of which a model is tested is also essential. It is just very precise measuring methods of spectra that have become the cause for questioning the adequacy of classical model of molecular structure of chemical compounds.[27] The revolution did not happen in the field of theory but in the precision of registration of spectra in the infra-red region and other wave lengths. Also important was the emergence of new techniques of experimental determination of molecular shape. The tremendous progress in the

field of experimental research led to the discovery of new facts that made chemists-theoreticians revise classical model of molecular structure and put forward several questions of key importance to the whole discipline of chemistry:[28] Is structure an intrinsic property of a molecule of a chemical compound? Is the model of molecular structure independent of the problem to the solution of which it is applied? Can all chemical phenomena, recognized as consequences of the molecular structure of a chemical compound, be inferred from a theoretical model of that structure? The negative answers to the above weakens the possibility of constructing a theoretical model of the molecular structure of a chemical compound understood as its essential attribute.

Before we pass on to the discussion of the breakthrough in the attitude of chemists-theoreticians towards the 'rigid' model of molecular structure, let us first note that both versions (the classical and quantum-classical) of the 'rigid' model meet fundamental requirements imposed on the notion of theoretical models by Achinstein (Sect. 1). They are sets of postulates that describe the structure of a certain type of physical objects (systems); they have an approximation character and are constructed within a conceptual apparatus of more general (basic) theories. It can be assumed that, apart from the explanative, predictive, heuristic, and educational functions, models of molecular structure serve the representative function as well. For to present a model of x is to present a way by which x is represented. Thus, although some chemists may accept an instrumentalist interpretation of models of molecular structures, the realistic interpretation could seem to be something natural. However, if one questions the existence of structure as an intrinsic molecular property, then one undermines at the same time the possibility of a theoretical model representing a 'rigid' and unchangeable structure of a molecule. Thereby one would threaten the account of the model of molecular structure as a structural one.

The basic assumptions for the new dynamic, also called 'soft model', are as follows: "a) rotational and vibrational motions cannot be separated; b) the coordinate system used for the description of these motions cannot introduce any redundant coordinates; c) the potential of the internal motions is semiempirical and, for many cases, is a function with a few minima."[29] In the dynamic model of a molecule, momentary positions of nuclei depend on the rotation of the molecule. It means that a change of the rotational state of a molecule induces a change of the vibrational states; and hence the interatomic distance depends on the rotational angular velocity. In this model, a local internal potential is described by the rotational-vibrational motions of the nuclei. In a high-resolution infrared spectrum, one can measure rotational-vibrational passages. Thus, we have to speak of rotational-vibrational molecu-

lar states. The rigid model of molecular structure may be applied only to low-excited rotational states.

While considering this problem, it is of great importance to bear in mind that the motion of the nuclei depends to a large extent, although not exclusively, on the electronic molecular state. Thereby the electronic structure is at least partially dependent on its interaction with the surrounding (*e.g.* on collisions with other molecules, the influence of electromagnetic and gravitational fields). In the discussed dynamic model, the shape of a molecule is no longer an intrinsic and fixed property, but a momentary property.

The dynamic model of molecular structure is a theoretical model in a different sense than the classical one. It is not constituted by theoretical postulates describing the way of determining the molecular shape, regarded as its intrinsic, unchangeable property. The dynamic model is worked out in a way that enables one to determine molecular shape as derivative from its energetic state that changes in time and depends on its interaction with the surrounding. Thereby the very notion of molecular structure, and first of all of molecular shape, loses its original sense and becomes a metaphor that does not represent any constant molecular property. Molecular structure changes in time and depends on a number of already mentioned conditions.

Within the dynamic model, molecular structures are not determined by a set of theoretical postulates that can be subject to axiomatization and formalization. Rules of generating these theoretical models become extremely complex and to speak about these models as about semantic ones is to lose any sense at all. What dominates is the belief that they cannot be derived from the fundamental postulates of quantum mechanics.[30]

The application of a specific model of molecular structure depends on the kind of experiments that we want to describe by the use of a model. With respect to many types of chemical experiments, classical ('rigid') models of chemical structure still perform their explanative, predictive, and heuristic function quite well. However, the model's representational function in the structural sense is called into question because, from the point of view of the dynamic model, regarding the structure as a molecular property is bound to many idealizing assumptions. Among chemists-theoreticians there begins to dominate an instrumentalist-pragmatic attitude towards theoretical models of molecular structure. The structure (molecular shape) "is such a useful property that it should not be abandoned; what is needed is just the awareness, though, that it is not a molecular attribute and it can be modified together with any change of its energetic state".[31] It can also be said – following J.L. Ramsey – that molecular structure (shape) is not an intrinsic property, but a response property. In addition, the same 'response' property may possess different representations, depending on experimental and measuring circumstances.

The belief that the dynamic model of molecular structure cannot be seen as a structural model but merely as an informational one seems to be justified in face of arguments presented in the present paper. Accepting the dynamic model, one has to reject constructive realism – both in its extreme version as well as in its moderate one, defended by Giere – with respect to the possibility of representing the real molecular structure. It has to be stressed, though, that it is just from the point of view of the dynamic model that it is possible to determine situations in which the rigid model of molecular structure will serve heuristic, explanatory and predictive functions in experimental chemistry.

Notes

[1] See Wójcicki 1979, p. 38.

[2] The application of semantic models in empirical sciences was discussed by *e.g.* Apostel 1961 and Przełęcki 1969.

[3] See Achinstein 1968, pp. 203-5.

[4] The necessity to regard the theoretical model in relative terms of the problem studied and the degree of precision of its solution is stressed by Wójcicki 1995/96a, pp. 398-404.

[5] The issue of conceptualization of the empirical system investigated was discussed in detail by Wójcicki 1979, pp. 37-41.

[6] See Wójcicki 1995/1996b, p. 510. The distinction between referential interpretation of the language of the empirical theory and procedural interpretation of terms occurring in the theoretical model built on the grounds of this theory was introduced by R. Wójcicki. He also demonstrated that the concept of procedural interpretation can, with certain reservations, be seen as a variation of the concept of semantic interpretation introduced by A. Tarski; *ibid.*, pp. 510-4.

[7] The above ambiguity was shown *e.g.* by Giere 1994, p. 75-98.

[8] See Giere 1985, p. 80.

[9] See van Fraassen 1980, pp. 11-9; 1984, 250-9.

[10] See *e.g.* Barnes 1977, p. 10; Bloor 1984, pp. 75-94.

[11] The distinction between representing and intervening was introduced and discussed by Hacking (1983).

[12] See *e.g.* Latour & Woolgar 1986 and papers in Lynch & Woolgar 1990.

[13] See Woolgar 1993, p. 33.

[14] *Ibid*., pp. 30-9.

[15] The meaning of these notions and a set of features by which the structure of a chemical compound is characterized were accepted by IUPAC. See Zeidler & Sobczyńska 1994, p. 183.

[16] See Konarski 1984, p. 622.

[17] See Mulckhuyse 1961, p. 134.

[18] The axiomatization and formalization of classical structure theory in the first-level language was presented by Mulckuyse 1961, pp. 135-51.

[19] *Ibid.*, pp. 142-151.

[20] See *e.g.* Vermeeren 1986.

[21] See Konarski 1994a, pp. 708-9.

[22] See Woolley 1991, p. 17; and about the same problem *e.g.* Woolley 1978, pp. 1073-8; Primas 1983, pp. 335-42.

[23] See Konarski 1984, p. 623.

[24] For details, see Konarski 1984, pp. 625-6.

[25] See Löwdin 1991, p. 14.

[26] See Konarski 1984, p. 626

[27] See Papousek & Aliev 1982; Maki *et al.* 1990, pp. 224-9 and references therein.

[28] These questions were formulated by Weininger 1984, p. 939.

[29] See Konarski 1994b, p. 439; for quantum chemistry beyond the Born-Oppenheimer approximation, see *e.g.* Woolley 1991, Löwdin 1991, Konarski 1987, 1992, 1994b, and references cited therein.

[30] The problem of the reduction of theory of chemical structure to quantum chemistry is currently widely discussed; see *e.g.* Amann 1992, 1993, 1996 and Weininger 1984. The criticism of the rigid model of molecular structure is generally associated with antireductionist attitude. Its account from the point of view of the dynamic model requires detailed discussion; see *e.g.* Primas 1983 and Ramsey 1997.

[31] See Konarski 1984, p. 632.

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