CROATICA CHEMICA ACTA CCACAA **70** (3) 777–786 (1997)

ISSN-0011-1643
CCA-2452

Conference Paper

On the Concept of a Chemical Model

Sonja Nikolić and Nenad Trinajstić

The Rugjer Bošković Institute, P.O.B. 1016, 10001 Zagreb, Croatia

Received August 19, 1996.; revised December 10, 1996.; accepted December 13, 1996

»Models are just that: models.«
N. Bhushan and S. Rosenfeld[1]

The concepts of model and modeling are discussed. Various classifications of models are given. It is pointed out that the progress of science in general and chemistry in particular is based on models and modeling since no better tools have yet been found to study Nature.

INTRODUCTION

In this report, we wish to discuss two concepts of importance for science in general and for chemistry in particular. These are the concept of the model and the concept of modeling as the process of model building.[2–5]

The word model is simply a technical term. It is derived from the Latin word *modulus* which is literally translated as a 'small measure'. The word model has very many meanings. Below we list all terms that one can find under the word model in two dictionaries, one American and one English, which are used by students. This is done in spite of the iconoclastic statement »*A dictionary is not a good source for understanding the meanings of a word, for the reason that it's likely to be apostolic*« by a leading anthropologist and social biologist Ashley Montagu.[6] First we give all terms found in »Webster's Ninth New Collegiate Dictionary«:[7]

(1) a set of plans for a building;
(2) copy, image;
(3) structural design;
(4) a miniature representation of something; also: a pattern of something to be made;
(5) an example for imitation or emulation;

(6) a person or thing that serves as a pattern for an artist; especially: one who poses for an artist;
(7) archetype;
(8) an organism whose appearance a mimic imitates;
(9) one who is employed to display clothes or other merchandise: mannequin;
(10) a: a type or design of clothing, b: a type or design of product (as a car);
(11) a description or analogy used to help visualize something (as a atom) that cannot be directly observed;
(12) a system of postulates, data and inferences presented as a mathematical description of an entity or state of affairs;
(13) version.

The second dictionary that we consulted was »Oxford Advanced Learner's Dictionary of Current English«.[8] In this dictionary, we have also found many terms under the word model. These are listed below:
(1) small-scale reproduction or representation of an object; design to be copied;
(2) person or thing to be copied;
(3) person or thing exactly like another;
(4) person who poses for sculptors, painters or photographers;
(5) person employed to wear clothes, hats, *etc.* so that prospective buyers may see them; mannequin;
(6) article of clothing, hat, *etc.* shown publicly by mannequins;
(7) design or structure of which many copies or reproductions are (to be) made;
(8) perfect, deserving to be imitated.

Terms from both dictionaries overlap to some extent, but they also point to the differences in the uses of the word model. However, the common feature of all uses of model may be summarized as follows: *A model is a representation of something else.*[9–11]

THE MODEL CONCEPT

The concept of the model is an essential device for all kinds of human activities including science and chemistry. One frequently tends to think, even in daily life, in terms of models though one may not be aware of this fact. Models are continuously devised and used because they possess many useful characteristics that are absent in the original, that is, models may be less expensive, more easily manipulated, more easily studied, more easily controlled, *etc.* than the original. A given theory is often nothing but the description and the use of a model. In the sciences and humanities, the validity of models is examined by logic and by experiments. If a model cannot explain the experiments, it must be revised or replaced by another which is able to explain them. This is indicative of the fact that most models have a limited life span. The revision of models and the introduction of novel models catalyzes the progress of science in general and of chemistry in particular. Actually, it would hardly be conceivable that any progress in the sciences could be made without the use of models and modeling. The competing models may be analyzed in terms of the principle of parsimony, popularly known as Ockham's Razor principle, according to which the simplest model is preferred.[12]

It is a scientific model that is a simplified representation of reality and the process by which the reality is imitated by a model is called modeling. The term *reality* is used here in a very broad sense. A model rarely reflects all the details of the reality it represents; for the sake of simplicity or transparency of the model, some details are left out. A more important function of such a model is to give us an idea of what reality is like. Another important function of a model is that certain tests and/or investigations can be performed upon the model more simply or more quickly or more economically than upon whatever the model represents. A model plane may be used to represent a jumbo-jet. In designing planes, or ships, or even automobiles much testing is done on models before the full-size device is constructed and tried in a real situation. Dolls are models of people. Children accept dolls as representing real people and often play with them by talking to them or pretending that dolls talk to them. Monkies (or many other animals) often serve as biological models for human medical research. One of the important features of a model is to reduce sometimes very complex systems to simpler ones while preserving their essential features. However, one may argue that a lesser complexity is not necessary for a model (though it may often incidentaly be). For example, for some space satellites, there is sometimes a duplicate satellite kept as a model to experiment with in case difficulties should develop. In this case, the aim is to have the complexity exactly the same, but in fact the model may be more complicated with various additional (non-obtrusive but weigth increasing) monitoring devices added to it, thereby making the model more complicated. Therefore, in place of complexity, one might instead imagine that what is really of relevance is something like accessibility (for the purposes of the experiment). Quite naturally, it is often the less complex system that is more accessible and which then is a model. It is worth noting that one model is sometimes based on another model. However, one point should be stressed: *There is no precise and unique definition of a model.* This is so because models often serve for quite different purposes and for different people they have different aims.

There are several important points about (scientific) models, which are summarized below:

(a) A model may differ considerably from the reality it represents.

(b) A model is often simpler than the reality it represents.

(c) For a given reality, there may be a number of models that could be useful. The simplest model could be selected, for example, by means of Ockham's razor criterion.

(d) Each type of model is ordinarily applicable to a set of different problems.

As it has been already stated, models are often used for certain definite purposes. In such a case, models may be classified as:[13]

(i) Logical

and

(ii) Epistemological.

Logical models enable certain inferences, which might not otherwise be possible to make. On the other hand, the epistemological models enable extension of human knowledge beyond known boundaries.

Depending on the method that is used to set up a model, one may distinguish pictorial, verbal, mathematical or computational (computer) models. All these models are used on the everyday basis in modern chemistry and elsewhere.[2–5,14–21]

Since the source of a model and the subject of a model may be the same or they may differ, models may be partitioned into two groups.[13] If the source of a model and the subject of a model are the same, the model is called a homeomorph. For example, a doll is a model of a baby and also modeled on a baby. When the source of a model and the subject of a model differ, the model is called a paramorph. For example, a structural formula is a model of a molecular structure, but is modeled on indirect observation because a molecule cannot be directly seen (at least at present). Both homeomorphs and paramorphs are used in science.

The use of models is essential for scientific thinking.[22] The two main uses of models in research are:

(a) heuristic

and

(b) explanatory.

The heuristic use of models is to simplify a phenomenon or to make it more readily handleable. The explanatory use of models appears in situations where the model is a model of the reality, then unknown.

A model must possess certain distinctive features. A useful model must be:[2,3,19]

(I) as simple as possible (a simple model is easier to remember than a complex model);

(II) portable (transferable);

(III) self-consistent (a model should not be contradictory and should be logically consistent);

(IV) stable (a model should be stable to small errors);

(V) flexible (easy to amend);

(VI) applicable as widely as possible (a model should be applicable, if possible, to a range of problems);

and

(VII) logically able to fail, granted only »low-level« models, or theories (that is, the model makes non-trivial predictions).

THE CLASSIFICATIONS OF MODELS

Models may be classified as[2,13,23] (I) iconic models, (II) analog models and (III) abstract (symbolic, conceptual) models. An iconic model closely resembles the physical form of the corresponding real object and mimics its functioning, but it differs in the scale and in dimension from the object (it could be smaller or bigger in size than the object it represents) and it is never called to function as its object does. For example, a structural formula of a molecule is an iconic model used by chemists all the time. Similarly, a model plane may be used to represent the latest fighter plane. Many models used in biosciences are iconic models. A monkey or a volunteer human being can be used to model a biological system for medical research. For instance, organ (heart, liver, lungs, *etc.*) transplantations were first performed on animals, and then, when the surgical techniques improved, on people. Although iconic models are mostly used in science and engineering, the term iconic is taken from the theory of arts (iconics = the science of images).[24] Paintings and geographic maps model 3D systems in two dimensions. The same is the case of the constitutional formula which is a 2D representation of the molecular 3D system. On the other hand, the double helix is a 3D model of the structure of DNA.

An analog model is similar to its object in its functioning and in its form. For example, the ball-and spring model of a molecular system, which is partly iconic, is at the same time an analog model of a molecule because it simulates molecular vibrations. It is the basis of the molecular mechanics method.[25] The analog computer models a mechanical system by changing the functions of capacitors, resistors and inductors for the functions of masses, springs and dashpots. There is no direct iconic similarity between the analog computer and its object, but the model is all the same a faithful image of the functioning of its object. Many models in biosciences are also analog in essence. For instance, pharmacological studies (*e.g.*, toxicities of drugs) on rats use the action of a drug on the biological system of a rat as an analog model for drug activity on human beings.

An abstract model is related to reality by symbols in a special way. For example, blueprints are abstract models: They bear an abstract likeness to buildings. It requires know-how to recognize the relationship between the abstract model (*e.g.*, the blueprint) and its object in reality (*e.g.*, the building) since they differ so much in many details and dimensions. Many models are in part or in whole abstract. Language is an abstract model. Similarly, the chemical nomenclature is also a highly abstract model used by chemists for oral, graphic and written communication. Nevertheless, it has been proven to be an extremely effective and useful model.[26,27] Mathematical chemistry offers a number of abstract models, many of which have appeared in this journal over the years.

Models are often partly iconic, partly analog and partly abstract. For example, the structural formula, which is one of the most important models in chemistry, is a model with the iconic, analog and large abstract contents. A good example to illustrate this point is the use of the truncated icosahedron to model the structure of buckminsterfullerene, a C_{60} carbon cluster, which is the parent molecule of the family of carbon cages named fullerenes which represent the third allotropic (and also the first molecular) form of carbon.[28] While the iconic and analog parts of the icosahedral picture of buckminsterfullerene are more or less evident, its abstract content might be hidden to some less mathematically-oriented chemists.[29]

Chemistry is primarily an experimental science and could be liberally defined as the science of molecules and their transformations.[30] However, the 19th century classical structural theory[31–33] and the 20th century quantum-chemical theory[32,34,35] turned chemistry into a science which has been readily mathematized.[36,37] Thus, models in chemistry can also be classified as (a) empirical models and (b) theoretical models. Empirical models are based on classical chemical ideas whose validity has been retained until today.[32] One of the most important empirical chemical models on which the whole foundation of chemistry rests is the model of molecular composition and structure. Namely, a molecule is modeled as an object made up from atoms of certain valencies which possess a characteristic spatial architecture. The structural formula has indeed a high information content based on experience and analogy.[38,39] This is the reason why chemists, upon only seeing a two-dimensional structural formula, can draw so many conclusions about the corresponding compound. However, the nature of chemical structure is still not quite understood.[40] Another important classical model of a timeless validity is the periodic system of elements, introduced by Mendeleev in 1869, whose basis was understood only after the quantum mechanics entered chemistry. There are too many empirical models used in chemistry to be mentioned here. The above two serve just as illustrations. Experimental chemists are trained[41] to skilfully use empirical models on a daily basis to rationalize their observations.

Theoretical models in chemistry can be classify as (A) quantum-chemical models, (B) more purely mathematical models and (C) computational (computer) models. These models serve usually to supply a more fundamental meaning to empirical models and sometimes to reduce the efforts of experimental chemists giving them hints on how to proceed in their research. There is no need to waste words on the usefulness of quantum-chemical models for the development of modern chemistry.[15,16,19,31–34,42,43] However, an overemphasis on quantum chemical computations may produce wrong ideas about the progress in chemistry. Thus, perhaps the most important chemist of this century Linus Pauling (1901–1994) warned us, near to the end of his life, with the following words:[44] »*We have, since 1927, people who make quantum mechanical calculations about molecules, molecular structures. Sometimes they get interesting results. A far more powerful method of thinking about chemical compounds is chemical structure theory. You can make much more progress with the empirical theory based upon a tremendous number of experimental facts than you can by making quantum mechanical calculations. No chemist in his laboratory working on organic, inorganic, or biochemical compounds makes any use of the quantum mechanical theory except in its qualitative aspects.*« This may be judged as an extreme point of view, but there is, undoubtedly, some truth in it.

Mathematical models, for example, based on the group theory[45] and graph theory[46,47] have also promoted our understanding of the basic principles on which the science of chemistry is founded. One of the referees has pointed out that mathematical models are models of problems associated with (chemical) reality but they do not directly characterize reality. This could be restated as: Mathematical models represent or identify a real-life situation or problem with a mathematical system. A good example to illustrate this is a reaction graph of any degenerate rearrangement. The vertices of this graph do not directly correspond to real molecules due to degeneracy. Nevertheless, the mathematical model of degenerate rearragements, realized by the reaction graph, provides very useful information about, for example, the minimum number of reaction steps needed to convert a chiral completely substituted derivative of a given molecule into its enantiomer. Živković has shown, for instance, that this number is 29 for a bulvallene molecule.[48]

Computers play an important role in contemporary chemistry. It is certainly much cheaper to run computer experiments before preparative efforts to investigate parameters such as stability, geometry, reactivity, *etc.* of a target compound in order to establish the simplest and the easiest route to make the compound.[5,14,16,19,49,50] Computer graphics can also give a three-dimensional model of the desired molecule and its spatial characteristics can likewise be a useful datum about the prospective compound. There is no doubt that the role of computers in chemical research in the future will dramatically increase. Nevertheless, the ultimate goal of chemistry, to make compounds, will continue to be the main occupation of chemists. However, it remains to be seen whether a person can be replaced by a computer guided robot in making compounds.

Models may also be classified as (a) qualitative models and (b) quantitative models. Most classical empirical models are qualitative models. Quantum-chemical models strive to be quantitative but, at the present level of theoretical and computational developments, they are at best semi-quantitative.

It has also been recently pointed out rather convincingly that essentially all models in chemistry are metaphorical models.[1] By this it is meant that at present chemists lack the knowledge and techniques to describe molecular-level entities and processes literally.

CONCLUDING REMARKS

More than 20 years ago Hall wrote an article entitled »*Modelling – A Philosophy for Applied Mathematicians*«.[51] We can only add to this that modeling has been a philosophy of chemistry since its beginnings – even alchemists used models in their work.[52] Why is it so? The answer was nicely put forward by Michael Dewar in 1984 in the following terse statement: »*We do not know, and probably never will know, what molecules are really like. Our understanding of them is based on* models *that reproduce their properties well enough to be useful*«. Therefore, one can state with certainty that models will remain to be the main tool in chemistry and in science, since so far we have not found any better and more efficient tool to study Nature. On that account, we wish to stress that model building, that is, modeling, is a challenging procedure which requires a lot of thoughtful and careful work.

Acknowledgement. – This work was supported in part by the Ministry of Science and Technology of the Republic of Croatia through Grant No. 1-07-159. We thank Professor Douglas J. Klein (Galveston, Texas) and Professor Carl Trindle (Charlottesville, Virginia) for constructive comments on early versions of this paper. We also thank the referees for their very useful comments.

REFERENCES

1. N. Bhushan and S. Rosenfeld, *J. Chem. Educ.* **72** (1995) 578–582.
2. C. Trindle, *Croat. Chem. Acta* **57** (1984) 1231–1245.
3. N. J. Turro, *Angew. Chem., Int. Ed. Engl.* **25** (1986) 882–901.
4. Z. B. Maksić, in: *Theoretical Models of Chemical Bonding.* Part 1: *Atomic Hypothesis and the Concept of Molecular Structure,* Z. B. Maksić (Ed.), Springer-Verlag, Berlin, 1990, pp. XIII–XXVIII.
5. I. Ugi, J. Bauer, C. Blomberger, J. Brandt, A. Dietz, E. Fontain, B. Gruber, A. von Scholley-Pfab, A. Senff, and N. Stein, *J. Chem. Inf. Comput. Sci.* **34** (1994) 3–16.

6. D. Brian, *Genius Talk – Conversations with Nobel Scientists and Other Luminaries,* Plenum Press, New York, 1995, p. 345.
7. *Webster's Ninth New Collegiate Dictionary*, Merriam-Webster, Inc., Springfield, MA, 1985, p. 762.
8. A. S. Hornby, A. P. Cowie, and A. C. Gimson, *Oxford Advanced Learner's Dictionary of Current English,* 23rd impression, University Press, Oxford, 1986, p. 544.
9. J. Malkevitch and W. Meyer, *Graphs, Models and Finite Mathematics,* Prentice-Hall, Inc., Englewood Cliffs, NY, 1974, p. 8.
10. G. Chartrand, *Graphs as Mathematical Models*, Prindle, Weber and Schmidt, Inc., Boston, 1977, p. 3.
11. W. R. Greco, *Bull. Math. Biol.* **48** (1986) 241–251.
12. R. Hoffmann, V. I. Minkin, and B. K. Carpenter, *Bull. Soc. Chim. France* **133** (1996) 117–130.
13. R. Harré, *The Philosophies of Science – An Introductory Survey*, University Press, Oxford, 1972.
14. G. Vernin and M. Chanon (Eds.), *Computer Aids to Chemistry*, Horwood/Wiley, New York, 1986.
15. N. Trinajstić (Ed.), *Mathematics and Computational Concepts in Chemistry*, Horwood/Wiley, New York, 1986.
16. Z. B. Maksić (Ed.), *Modelling of Structures and Properties of Molecules,* Horwood/Wiley, New York, 1987.
17. M. Marsili, *Computer Chemistry*, CRC Press, Boca Raton, FL, 1990.
18. M. A. Johnson and G. M. Maggiora (Eds.), *Concepts and Applications of Molecular Similarity,* Wiley, New York, 1990.
19. Z. B. Maksić (Ed.), *Theoretical Models of Chemical Bonding*, Springer-Verlag, Berlin, 1990, a 4-volume set.
20. I. Ugi, J. Bauer, K. Bley, A. Dengler, A. Dietz, E. Fontain, B. Gruber, R. Herges, M. Knauer, K. Reitsam, and N. Stein, *Angew. Chem., Int. Ed. Engl.* **32** (1993) 201–227; see also S. Reichelt, A. Reichelt, N. Müller, and I. Ugi, *Croat. Chem. Acta* **69** (1996) 813–825.
21. D. Bonchev and O. Mekenyan (Eds.), *Graph Theoretical Approaches to Chemical Reactivity,* Kluwer Academic Publishers, Dordrecht, 1994.
22. R. Harré, *The Principles of Scientific Thinking*, University Press, Chicago, 1970.
23. N. Trinajstić, in: *MATH / CHEM / COMP 1987,* Graovac A. (Ed.), Elsevier, Amsterdam,1988, pp. 83–100.
24. *e.g.,* J. Bialostocki, *History of Arts and Humanistic Science* (in Croatian, translation from Polish), GZH, Zagreb, 1986.
25. U. Burkert and N. L. Allinger, *Molecular Mechnics*, ACS, Washington, 1982; see also P. Comba and T. W. Hambley, *Molecular Modeling, VCH,* Weinheim, 1995.
26. D. J. Polton, *Chemical Nomenclatures and the Computer*, Wiley, New York, 1993.
27. *e.g.*, M. Randić, S. Nikolić, and N. Trinajstić, *J. Chem. Inf. Comput. Sci.* **35** (1995) 357–365.
28. H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley, *Nature* **318** (1985) 162–163.
29. *e.g.*, N. Trinajstić, M. Randić, D. J. Klein, D. Babić, and Z. Mihalić, *Croat. Chem. Acta* **68** (1995) 241–267.
30. R. Hoffmann, *Amer. Scientist* **78** (1990) 14–15.
31. C. A. Russell, *The History of Valence*, University Press, Leicester, 1971.
32. D. J. Klein and N. Trinajstić, *J. Chem. Educ.* **67** (1990) 633–637.

33. W. H. Brock, *The Fontana History of Chemistry*, Fontana Press, London, 1992
34. H. Eyring, J. Walter, and G. E. Kimball, *Quantum Chemistry*, 10th printing, Wiley, New York, 1961.
35. C. A. Coulson,*Valence*, 2nd edition, University Press, Oxford, 1961.
36. J. Karle, *J. Chem. Inf. Comput. Sci.* **34** (1994) 381–390.
37. N. Trinajstić, *Mathematics and Chemistry – The Unlikely Partners*, Research Studies Press Ltd, Taunton, Somerset, 1997, pp. 17–39.
38. J. W. Cornforth, *Austral. J. Chem.* **46** (1993) 157–170.
39. D. H. Rouvray, *J. Chem. Inf. Comput. Sci.* **34** (1994) 446–452.
40. M. Randić, *J. Chem. Educ.* **69** (1992) 713–718.
41. *e.g.*, T. L. Brown, H. E,. LeMay, Jr., and D. E. Bursten, *Chemistry – The Central Science,* 5th edition, Prentice Hall, Englewood Cliffs, 1991.
42. R. B. Woodward and R. Hoffmann, *The Conservation of Orbital Symmetry,* Verlag Chemie, Weinheim, 1970.
43. D. J. Klein and N. Trinajstić (Eds.), *Valence Bond Theory and Chemical Structure,* Elsevier, Amsterdam, 1990.
44. Ref. 6, p. 23.
45. D. Bonchev and Rouvray (Eds.), *Chemical Group Theory – Introduction and Fundamentals*, Gordon & Breach, Amsterdam, 1994.
46. D. Bonchev and D. H. Rouvray (Eds.) *Chemical Graph Theory – Introduction and Fundamentals,* Abacus/Gordon & Breach, New York, 1991.
47. N. Trinajstić, *Chemical Graph Theory*, 2nd revised edition, CRC Press: Boca Raton, FL, 1992.
48. T. Živković, Report at *MATH / CHEM / COMP 1996,* an International Course and Conference on the Interfaces between Mathematics, Chemistry and Computer Science, Dubrovnik, Croatia, June 24–28, 1996; see also T. P. Živković, *Croat. Chem. Acta* **69** (1996) 215–222
49. E. J. Corey and X.-M. Cheng, *The Logic of Chemical Synthesis*, Wiley, New York, 1989.
50. R. Carlson and A. Nordahl, *Topics Curr. Chem.* **166** (1993) 3–64.
51. G. G. Hall, *Bull. Inst. Math. Appl.* **9** (1972) 226–228.
52. F. Sherwood Taylor, *The Alchemists*, Paladin, Frogmore, St Albans, Hearts, 1976.

SAŽETAK

O koncepciji kemijski model

Sonja Nikolić i Nenad Trinajstić

Razmatrane su koncepcije modela i modeliranja. Dana je klasifikacija modela. Istaknuto je da se napredak cijele znanosti, ne samo kemije, temelji na modelima i modeliranju, jer za sada nisu pronađeni bolji pristupi proučavanju prirode.