Dori, Y., & Barak, M. (2000). Computerized Molecular Modeling: Enhancing Meaningful Chemistry Learning. In B. Fishman & S. O'Connor-Divelbiss (Eds.), *Proceedings of the Fourth International Conference of the Learning Sciences* (pp. 185-192). Mahwah, NJ: Erlbaum.

Computerized Molecular Modeling: Enhancing Meaningful Chemistry Learning

Yehudit Judy Dori[1, 2] and Miri Barak[2]
[1] Center for Educational Computing Initiatives, Massachusetts Institute of Technology
Cambridge, MA 2139-4307, USA
Fax: 617-253-8632
Email: dori@ceci.mit.edu
[2] Department of Education in Technology and Science, Technion, Israel Institute of Technology
Haifa 32000, Israel
Fax: 972-4-8325445
Email: bmiriam@techunix.technion.ac.il

Abstract: Model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students. To alleviate these problems we have introduced an innovative teaching/learning approach that employs a combination of virtual and physical models in an organic high school chemistry curriculum. We studied the effect of this approach on enhancing meaningful learning in chemistry. Experimental group students were more capable of defining and implementing new concepts in organic chemistry than their control group counterparts. When required to explain their answers, most of the experimental group students used mainly sketches of ball-and-stick models and some space-filling models. Experimental group students understood the model concept better and were more capable of applying transformation from one-dimensional to two- or three-dimensional molecular representations and vice versa.

Keywords: modeling/models, visualization, learning environment, science education

Theoretical Background

Chemistry students find it hard to connect among the molecular formula, the geometric structure and the molecule characteristics (Gabel & Bunce, 1994; Johnstone, 1991). Understanding the particulate nature of matter, interpretation of symbols and visualizing spatial structures of molecules are essential skills students need for solving problems in chemistry in general and in organic chemistry in particular (Barnea & Dori, 1999; Dori, 1995; Dori & Hameiri, 1998). Many students experience difficulties in understanding topics related to organic compounds (Brook, 1988; Ryles, 1990; Schmidt, 1992; Shani & Singerman, 1982; Simpson, 1983; Whitfield, 1968). These difficulties are explained by the need of students to learn many concepts, theories and processes (Brook 1988; Simpson, 1983).

Scientists, engineers and science educators use models to concretize, simplify and clarify abstract concepts, as well as to develop and explain theories, phenomena and rules. An important value of models in science and science education is their contribution to visualization of complex ideas, processes and systems. A virtue of a good model is that it stimulates its creators and viewers to pose questions that take us beyond the original phenomenon to formulate hypotheses that can be examined experimentally (Bagdonis & Salisbury, 1994; Hardwicke, 1995; Raghavan, & Glaser, 1995; Toulmin, 1953). Gilbert and Boulter (1998) distinguish between target systems, mental models, expressed models, consensus models and teaching models. Other researchers underscored the need for models as enablers of students' mental transformation from two-dimensional to three-dimensional representations (Baker & Talley, 1974; Barak & Dori, 1999; Eliot & Hauptmam, 1981).

One of the problems that arises while using concrete models is that insufficient emphasis is placed on the fact that models are theory-based simulations of reality. Teachers and students should, therefore, be made aware of the fact that models, employed in a variety of research, study and design contexts, are not complete representations of the realities they are supposed to represent (Osborne & Gilbert, 1980).

Applied to chemistry, physical ball and stick models derived from polystyrene spheres and plastic straws are not merely enlargements of the molecules they are intended to represent. These are analogue models that are used to explain new and abstract concepts. Some of the properties are similar to aspects of the target they are representing. For example, the relative diameter of the spheres represents the size of the different atoms. Other aspects, however, are not reflected in the model. For example, in a ball-and-stick model type, all sticks (straws) are of equal length, while "real" molecular bond lengths are not. Other models focus on different properties of the molecule, thereby creating multiple modes of representing the same molecule. Teachers frequently use just one type of model, limiting students' experience with models and causing their model perceptions to be partially or completely inadequate (Barnea & Dori, 2000).

The use of concrete molecular models to illustrate phenomena in chemistry teaching has been widespread for a relatively long time (Peterson, 1970). The choice of model type has an impact on the image students create concerning the ways in which particles are shaped and how they function in the "real" world from a scientific viewpoint. Theoretical chemists, experimentalists and educators are taking advantage of computerized environment in order to stimulate different model types quickly and efficiently (Kozma, 1999; Wilson 1997). Information technology helps relieving present-day researchers and students from the laborious task of data collection and enables them to engage in creative thinking and problem solving. The development of computerized molecular modeling (CMM) made traditional models less favorable in the late 1960's. Not only are computers capable of drawing and manipulating molecules in three dimensions. They are also powerful tools for predicting molecular spatial structure through energy minimization calculations based on quantum mechanics. These capabilities have opened the way for advanced research in chemistry, resulting, among other things, winning Nobel Prize in chemistry (1998).

Among the advantages of using innovative technology in science education are the options of providing for individual learning, simulation, graphics, and the demonstration of models of the micro and macro world (Dori & Barnea, 1997; Krajcik, Simmons & Lunetta, 1988; Krieger, 1996). Students need more experience with models as intellectual tools that provide contrasting conceptual views of phenomena, and more discussion of the roles of models in the service of scientific inquiry (Gabel & Sherwood, 1980; Grosslight, Unger, Jay & Smith, 1991). Most educators use a limited number of static models, and do not emphasize the way in which models are created, their essential role in science learning, or their advantages and limitations (Gilbert, 1997). Williamson and Abraham (1995) studied the effect of computer animations on college student mental models of chemical phenomena. The researchers argued that the animations helped students understand the subject matter better while improving their ability to construct dynamic mental models of chemical processes.

Research Objective, Settings and Population

Our research objective was to investigate the effect of using various types of models on student understanding of new concepts and the spatial structure of molecules, their preference of a particular model type and modes of explanation. The teaching method combined physical (plastic) and virtual (computerized) three-dimensional molecular models. The combination of physical and virtual model types was designed to benefit from advantages of each type while the complementary type compensates for its disadvantages. The research population consisted of 276 students from nine high schools in Israel. The experimental group consisted of 154 students who studied according to the innovative method. The control group consisted of 122 students who studied in a traditional method. Control group teachers used models only rarely, and only for demonstration. The research tools included a designated learning unit, computerized molecular modeling software and database, and pre- and post-course questionnaires on organic compounds and models. The science education research team developed and improved the learning materials and the questionnaires. The learning materials were aimed at encouraging students to use different types of models for building spatial structures of organic molecules (Dori & Barak, 1999).

Research Results

Students' answers to the pre-model and pre-organic compound questionnaires were analyzed and scores were summarized. The average score of the experimental group was compared to the average score of the control group and analyzed for randomness of the class effect in this research. The results showed that in the pre-model questionnaire there was no significant class effect while in the pre-organic compound questionnaire a significant class effect was found ($Z=2.01$, $p=0.0450$). No significant differences were found between experimental and control students in the pre-model questionnaire and in the pre-organic compound questionnaire. Nonetheless, the pre-course questionnaires served as covariant in the Mixed Model Procedure (Littell, Milliken, Stroup & Wolfinger, 1996) for analyzing the post-questionnaires results. The new teaching method was determined as the fixed effect and the class was determined as the random effect. The students' scores in the pre-course questionnaires also served for categorizing students from each research group into three academic levels: high, intermediate and low.

The Organic Compound Questionnaire

The organic compound questionnaire was designed to determine whether and to what extent the new teaching method improves concept understanding and bi-directional transformations. We also examined students' preference for a particular model type.

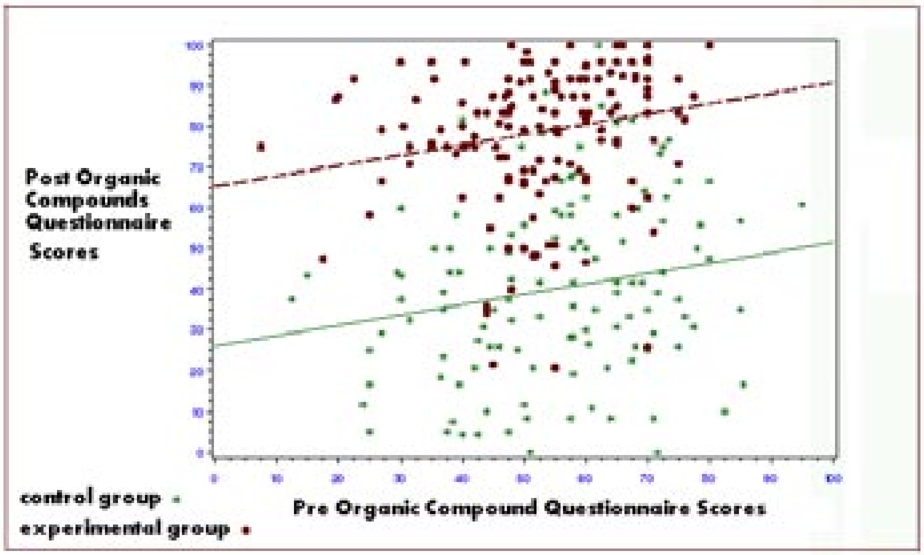

Figure 1. Regression lines for organic compound questionnaire

Figure 1, which presents the regression lines for the organic compound questionnaire, shows a steady gap between the experimental and control group scores. The gap is in favor of the experimental group and is statistically significant ($t = -17.12$, $p < 0.00001$). To examine the effect of the learning method on students' ability to carry out bi-directional transformations between one- and two- or three-dimensional representations, we performed an in-depth analysis of individual problems that were presented to the students in the post-organic compound questionnaire. The two significant factors, which were found to explain the higher performance of the experimental student scores for these problems were the pre-course questionnaire score ($F = 171.3$, $p = 0.001$) and the research group ($F = 6.8$, $p = 0.01$).

Another research aspect we addressed was the different modes students used to explain their answers in the question that dealt with identifying models and isomers in the organic compound questionnaire. Three modes of explanations were defined: textual, graphic and a combination of the two. The assumption was that the experimental group students, who learned by the new teaching method, used physical and virtual models and drew them, would provide explanations that are expressed graphically or in a combination of text and graphics. Indeed, Table 1 shows a significant difference between the research groups regarding their modes of explanation. The Wilcoxon 2-sample test (Mann Whitney) shows a significant difference between the research groups for all three academic levels combined. This difference implies that students in the experimental group were capable of providing more explanations in all three modes (textual, graphic and the combination of both) than students in the control group.

To characterize the differences within each research group individually, frequencies of the three modes of explanation were calculated. Figures 2 and 3 show the different modes of explanation by academic levels among experimental group students and control group students, respectively.

Table 1. Comparison of research groups regarding modes of explanation

Modes of Explanation	Mann Whitney	
	Z	p
Textual	3.78	0.0002
Graphic	7.07	0.0001
Combination	2.42	0.0154

The results clearly show that the gap, which had existed in the pre-course organic questionnaire, between high and low academic students was almost closed for the experimental students. The corresponding gap for the control group, however, was still noticeable. In particular, over 60% of both low and intermediate academic level students could still not provide any explanation whatsoever. In the experimental group only less than 20% of the corresponding academic levels did not provide any explanation.

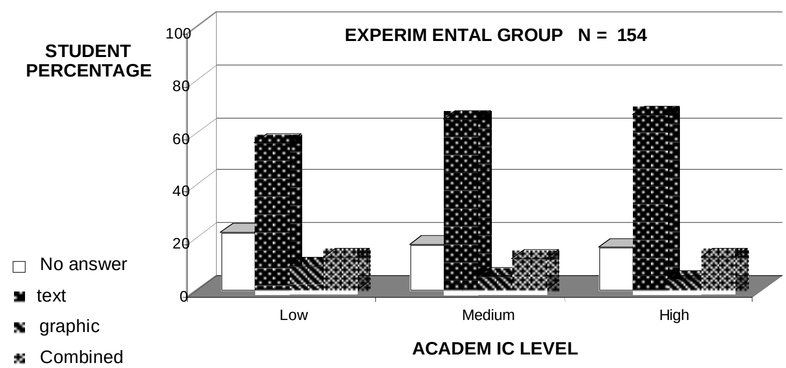

Figure 2. Characterizing different modes of explanation by student academic levels among experimental group students

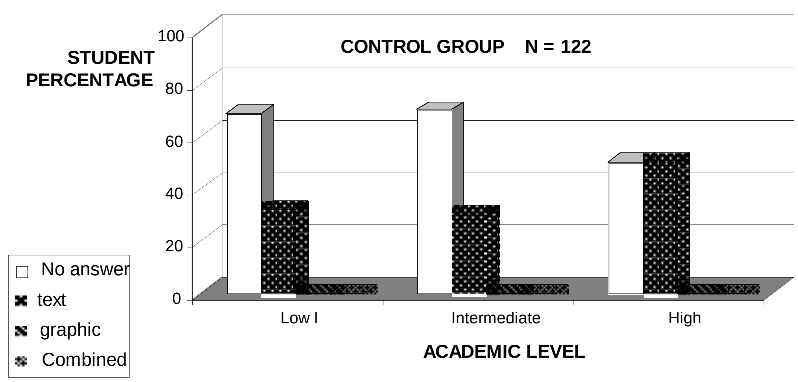

Figure 3. Characterizing different modes of explanation by student academic levels among control group students

To investigate students understanding and implementation of the three representation modes, we looked into their ability to carry out bi-directional transformations between two/three dimensions and one dimension, and the ability to identify/draw isomers of a given molecule. Table 2 summarizes the results. Experimental group students scored higher than their control group counterparts, demonstrating the contribution of incorporating virtual and physical molecular models into organic chemistry.

To gain insight into the specific types of model students preferred to use in their explanations, we analyzed the question that dealt with bi-directional transformations between one- and two-dimensional representations.

Table 2. Understanding and applying representation modes by research groups

Modes of Representation	DF	t	p
Wireframe	134	4.59	0.0001
Ball and Stick	106	6.14	0.0001
Space Filling	111	7.79	0.0001

Figures 4 and 5 show the distribution of preferred model representation for the experimental and control student groups, respectively. The results for each group are presented separately for each one of the three academic levels - low, intermediate and high.

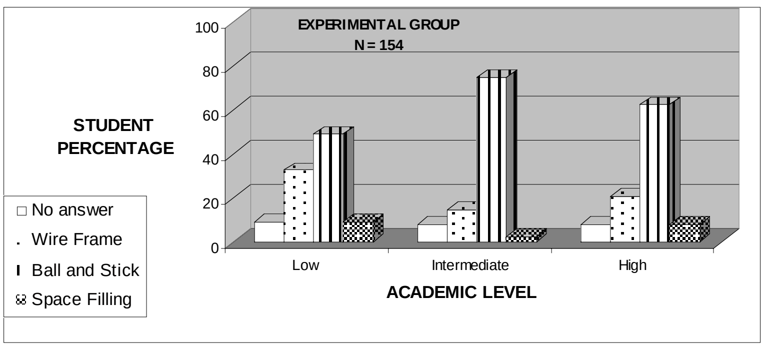

Figure 4. The experimental group preferred model representation mode

As Figure 4 shows, the experimental students favored the ball-and stick, followed by wireframe model type. Only few used the space-filling model or did not respond to this question at all. About half of the control students, on the other hand, chose not to respond to this question. Most of those who did respond used wireframe, as Figure 5 shows. A possible explanation to this difference in model type preference can be attributed to the similarity of the wireframe representation to the structural formulae, which the conservative teaching style employs. The results were found to be statistically significant by the Mann-Whitney test for each one of the three representation modes ($p < 0.0001$).

The Model Questionnaire

The model questionnaire was designed to find out how the new teaching method contributes to the understanding and applying of the model concept. The average score of the experimental group was compared to the average score of the control group. The statistical analysis of the results shows a high significant difference between the research groups. The experimental group students defined the model concept better and they were able to identify model characteristics and their functions better ($F=38.23$, $p=0.0001$).

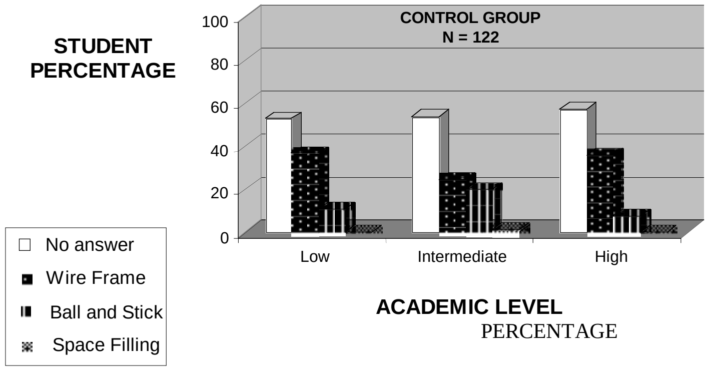

Figure 5. The control group preferred model representation mode

A pattern similar to the regression lines for the organic compound questionnaire (Figure 1) was obtained also for the model questionnaire. It too shows a constant gap between the experimental students scores (regression line intercept = 46.8) and control students scores (intercept = 29.0). The gap is in favor of the experimental group and is statistically significant ($t = -6.18$, $p < 0.0001$).

We compared the research groups regarding their ability to apply transformations among four chemistry understanding levels: symbol, macro, micro and process. Figure 6 shows that the average score of the experimental group students at all three academic levels was higher than that of the corresponding academic levels of the control group students. Figure 6 also shows that students, who were classified in the pre model questionnaire as having intermediate or low academic level, succeeded in narrowing the gap between them and the high achievers by scoring high in the post questionnaire.

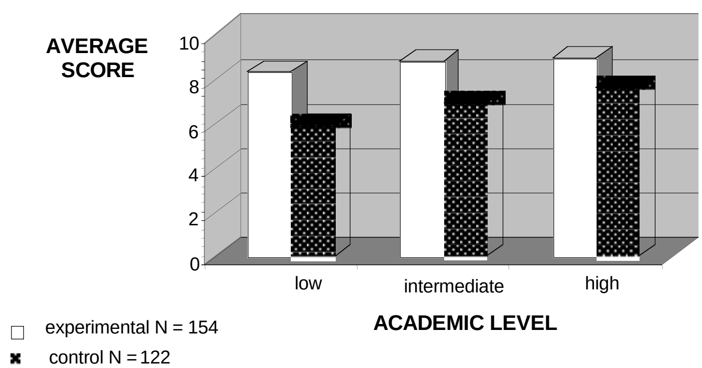

Figure 6. Post model questionnaire average score for transformation ability among four chemistry understanding levels

Table 3. Comparing research groups regarding transformation ability among chemistry understanding levels

Transformation Ability	**Mann Whitney**	
	Z	**p**
High	2.60	0.009
Intermediate	3.90	0.0001
Low	4.67	0.0001

Discussion and Summary

Interpretation of symbols, as well as understanding the particulate nature of matter and spatial structures are essential skills students need for solving problems in organic chemistry. Students at all levels find chemistry one of their more difficult courses at the secondary level (Gabel, 1998). Several review studies (Gabel & Bunce, 1994; Krajcik, 1991; Stavy, 1995) suggested that science educators and teachers need to promote conceptual understanding and non-algorithmic problem solving methods. Other scholars argued that chemistry educators need to examine teaching strategies that help students gain better scientific concept understanding accepted by the scientific community (Treagust, Duit & Fraser, 1996).

Model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students (Dori, 1995; Dori & Barak, 1999). To alleviate these difficulties we have presented an innovative teaching/learning approach. Until recently, scientists and researchers almost exclusively used computerized molecular modeling. In this study we introduced both virtual and physical models in an organic chemistry curriculum and studied their effect on enhancing meaningful learning in chemistry. 276 students from nine high schools in Israel participated in this study. Research tools included a designated learning unit, computerized molecular modeling software and database, and pre- and post-course questionnaires on organic compounds and models.

Experimental group students were more capable of defining and implementing isomerism and functional group concepts than their control group counterparts. When required to explain their choices, most of the experimental group students used mainly sketches of ball-and-stick models and some space-filling models. Most students of the control group did not provide any explanation (although required to do so) and those who did, used mainly 2-D wireframe model that resembles their teacher's chalk and board structural formulae. Experimental group students understood the model concept better and were more capable of applying transformation from one-dimensional to two- or three-dimensional molecular representations and vice versa. Based on these results, we recommend incorporating a combination of virtual and physical models in chemistry teaching/learning as a means to foster meaningful learning and spatial understanding of molecular structure.

References

Bagdonis, A.S., & Salisbury, D.F. (1994). Development and validation of models in instructional design. *Educational Technology, 34,* 26-32.

Baker, R.S. & Talley, H.L. (1974). Visualization skills as a component of aptitude for chemistry - A construct validation study. *Journal of Research in Science Teaching, 11*, 95-97.

Barak M. & Dori, Y.J. (1999). Model perception and understanding the spatial structure of organic molecules by high school chemistry students. *Science Teachers Education toward the New Millennium*, Technion, Haifa, Israel.

Barnea, N. & Dori, Y.J. (1999). High school chemistry students' performance and gender differences in a computerized molecular modeling learning environment. *Journal of Science Education and Technology, 8*, 4, 257-271.

Barnea, N., & Dori, Y.J. (2000). Computerized molecular modeling the new technology for enhancing model perception among chemistry educators and learners. *Chemistry Education: Research and Practice in Europe, 1*, 1, 109-120. http://www.uoi.gr/conf_sem/cerapie/pdf/16barneaf.pdf.

Brook, D. W. (1988). Science education notes: The teaching of organic chemistry in school - Can we learn from the Kenyan experience. *School Science Review, 69*, 248, 575 - 578.

Dori, Y.J. (1995). Cooperative development of organic chemistry computer assisted instruction by experts, teachers and students. *Journal of Science Education and Technology, 4,* 2, 163-170.

Dori, Y.J., & Barak, M. (1999). Computerized molecular modeling as a collaborative learning environment. *Computer Supported Collaborative Learning - CSCL99* (pp. 142-150). Stanford University, Palo Alto, CA, USA. http://kn.cilt.org/cscl99/A16/A16.HTM

Dori, Y.J., & Barnea, N. (1997). In-service chemistry teachers training: the impact of introducing computer technology on teachers attitudes and classroom implementation. *International Journal of Science Education, 19*, 577-592.

Dori, Y.J. and Hameiri, M. (1998). The "Mole Environment" studyware: Applying multidimensional analysis to quantitative chemistry problems. *International Journal of Science Education, 20*, 3, 317-333.

Eliot, J.K., & Hauptmam, A. (1981). Different dimensions of spatial ability. *Studies in Science Education, 8*, 45-66.

Gabel, D. (1998). The complexity of chemistry and implications for teaching. In B.J. Fraser & K.G. Tobin (Eds.). *International Handbook of Science Education* (pp. 53-66). Kluwer Academic Publisher, Dordrecht/Boston/London.

Gabel, D. & Bunce, D.M. (1994). Research on problem solving: Chemistry. In D. Gabel (Ed.). *Handbook of Research on Science Teaching and Learning* (pp. 301-326). Macmillan, New York.

Gabel, D., & Sherwood, R. (1980). The effect of student manipulation of molecular models on chemistry achievement according to Piagetian level. *Journal of Research in Science Teaching, 17,* 75-81.

Gilbert, J.K. (1997). *Exploring models and modeling in science and technology education*. The University of Reading, The New Bulmershe Papers, UK.

Gilbert, J.K., & Boulter, C.J. (1998). Learning science through models and modeling. In B.J. Fraser & K.G. Tobin (Eds.). *International Handbook of Science Education* (pp. 53-66). Kluwer Academic Publisher, Dordrecht/Boston/London.

Gilbert, S.W. (1991). Model building and a definition of science. *Journal of Research in Science Teaching, 28,* 73-79.

Grosslight, L., Unger, C., Jay, E., & Smith, C.L. (1991). Understanding models and their use in science: conceptions of middle and high school students and experts. *Journal of Research in Science Teaching, 28*, 9, 799-822.

Hardwicke, A.J. (1995). Using molecular models to teach chemistry. Part 1: Modeling molecules. *School and Science Review, 77*, 59-64.

Johnstone, A.H. (1991). Why is science difficult to learn? Things are seldom what they seem. *Journal of Computer Assisted Learning*, **7**, 75-83.

Kozma, R.B. (1999). Students collaborating with computer models and physical experiments. *Computer Supported Collaborative Learning - CSCL99.* Stanford University, Palo Alto, CA, USA. http://kn.cilt.org/cscl99/A39/A39.HTM

Krieger, J.H. (1996). New software kicks in. *Chemistry and Engineering News*, September, 30-40.

Krajcik, J.S. (1991). Developing students' understanding of chemical concepts. In S.M. Glynn, R.H. Yeany, & B.K. Britton (Eds.). *The psychology of learning science* (pp. 117-147). Lawrence Erlbaum, Hillsdale, New Jersy.

Krajcik, J.S., Simmons, E. R. & Lunetta, N. (1988). A research strategy for the dynamic study of students' conception and problem solving strategies using science software. *Journal of Research in Science Teaching, 25,* 147-155.

Littell, R.C., Milliken, G.A., Stroup,W.W. & Wolfinger, R.D. (1996). *SAS system for mixed models.* Cary, NC: SAS Institute Inc. North Carolina.

Nobel Web Site (1998). http://www.nobel.se/announcement-98/chemistry98.html

Osborne, R.J., & Gilbert, J.K. (1980) The use of models in science teaching. *The School and Science Review, 62*, 57-67.

Peterson, Q.R. (1970). Some reflections on the use and abuse of molecular models. *Journal of Chemical Education, 47*, 1, 24-29.

Raghavan, K., & Glaser, R. (1995). Model based analysis and reasoning in science: the MARS curriculum. *Science Education*, 79, 37-61.

Ryles, A.P. (1990). Teaching A-level organic chemistry mechanisms: Some suggestions. *School Science Review*, *72*, 258, 71-74.

Schmidt, H.J. (1992). Conceptual difficulties with isomerism. *Journal of Research in Science Teaching, 29,* 9, 995-1003.

Simpson, P. (1983). A new organic mythology. *Education in Chemistry*, 20, 5, 166.

Shani, A. & Singerman, A. (1982). A self-study, one paced basic organic chemistry course. *Journal of Chemical Education, 59*, 223-224.

Stavy, R. (1995). Conceptual development of basic ideas in chemistry. In S. Glynn & R. Duit (Eds.). *Learning science in the schools: Research reforming Practice* (pp. 131-154). Lawrence Erlbaum, Mahwah, NJ.

Toulmin, S. (1953). *The philosophy of science: An introduction.* Harper and Row, New York.

Treagust, D.F., Duit, R. & Fraser, B.J. (1996). *Improving teaching and learning in science and mathematics.* Teachers College Press, New York.

Whitfield, R.C. (1968). An evaluation of an electronic approach to organic chemistry in the sixth form. *School Science Review*, 50, 171, 315.

Williamson, V.M., & Abraham, M.R. (1995). The effects of computer animation on the particulate mental models of college chemistry students. *Journal of Research in Science Teaching, 32,* 521-534.

Wilson, E.K. (1997). Thinking instead of 'Cookbooking'. *Chemistry and Engineering News,* May, 33-34.