Playing with Molecular Models

Pierre Laszlo

Abstract: Any serious study of the uses of molecular models in chemistry has to mention play as an essential component. A research chemist will use them not unlike a young child playing with a toy: exploring their features, trying out their resilience, probing their innards, tinkering, day-dreaming, and thus finding out new avenues of adventures of the mind and in the laboratory. Reasons for such an assimilation of a molecular model to a toy are given and assessed critically.

Keywords: *molecular models*, *play*, *transitional object*, *toys*, *tinkering*.

1. Introduction

This article is a companion piece to earlier publications co-authored with Roald Hoffmann, dealing with the general topics of representation in chemistry,[1] with paradigmatic shifts ensuing from the correction of mistaken formulations of chemical compounds,[2] and with the role of conversation in science.[3]

To complement the special issues of HYLE dealing with models in chemistry with a paper on the playful aspects of model handling is as pleasant as it amounts to an internalized obligation, on the part of a practicing professional organic chemist. For this paper, I had no better choice than an eclectic method. I draw on several decades of personal experience with molecular models as a professional researcher (methodology of organic synthesis, spectroscopic studies of molecular interactions) and as an educator. I shall build my case with other components, too, culled from the histories of science, games, and pedagogy. There will be also psychological and sociological elements, to be handled critically and without undue reliance.[4]

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2. What is play?

Playing is an activity (truly, an intricate set of very diverse activities and behaviors) associated with children, but which of course also adults are occasionally engaged in, too.[5] When performed by young children, a play shows components of orienting within an environment; achieving a measure of control of the objects present; learning to associate *e.g.* visual and tactile perceptions; mimicking or emulating a behavior, typically that of adults in 'pretending games'; identifying the self and pitting it against others in social interactions. Most of these factors are also involved, are at play one might say, in the handling of molecular models by professional chemists.

Johann Huizinga in his justifiably classic book on play and games, *Homo ludens*,[6] emphasized the competition aspect. As a rationalist, he espoused the ages-old discrimination by contrasting the playful with the serious. Later, Roger Caillois[7] also put his systematic study of games under the same overarching duality. He went on organizing games according to a typology along the four basic categories of competition (*agôn*), chance (*alea*), altered mental states (*ilinx*), and simulation (*mimicry*). Clearly, playing with a model for representing a chemical compound belongs predominantly to the fourth category.

Furthermore, many languages (such as French) denote by a word such as *jeu* or the equivalent an imperfect fit in the adjustment of interacting mechanical parts, as in a geared assembly or in a piece of woodwork or carpentry. The real mechanical device is distinguished from the idealized fully deterministic contraption in the abstract realm of rational mechanics precisely by such a measure of freedom, by a degree of behavior unpredictable from the well-understood laws and rules of mechanics.[8] One might say that *jeu* in any kind of mechanical devices serves as a real-life and avowedly anthropomorphic metaphor, standing for this playful-serious duality.

True, quite a few authors have questioned its very existence. In the philosophical tradition of Nietzsche and Heidegger, Jacques Derrida for instance regards play as the cornerstone for any culture.[9] Derrida's interpretation of play as a cultural root also enjoys an ancient and distinguished history. To quote from the entry in the *Encyclopédie* for 'Game of Roman children (Roman history)':

> One of their most usual games was representation of a day at court, under all its aspects, which they named *judicia ludere*. There were judges, prosecutors, attorney, and guards to put in jail a condemned party. Plutarch, in his life of Cato from Utica, tells about one of these children who, after the ruling was led by a boy older than he was, took him to a small room and locked him up. The child was scared and called for Cato (also a participant in this game) to help him. Cato made his way through their playmates, freed his client, and brought him back to his place […].

Thus, Derrida's is quite a respectable viewpoint. Nevertheless, for the purpose of this paper the discussion will be set in the traditional rationalist interpretation.

Another feature yet ought to be mentioned in this section devoted to a reminder of the most relevant factors, for our purpose, in play and games. This is game as the attempted prediction of a random outcome. We can best illustrate this aspect with the Brazilian illegal lottery, *jogo do bicho*, originated in Rio de Janeiro. This occurred in the distant past, about a century ago: at irregular intervals, animals from the zoo were taken out for a stroll through the Rio streets. Soon, the Cariocas (inhabitants of Rio) started betting on which animals would show up. Thus, the *jogo do bicho*, a form of gambling, had been invented. It endures to this day. There is a total of 24 emblematic animals. The results of the daily draw are posted in every bar. Brazilians are very fond of their game, both on account of it being illegal (most people, worldwide, when playing games, such as cowboys and Indians, prefer the side of the outlaws to that of the law enforcers, the cops) and for the connection it enables them to draw between their dream life and reality (one of them might say: "I dreamt of hearing mocking sounds in the forest, hence I'll wager on the monkey."). As Émile Borel has reminded us most convincingly,[10] all such money games are structurally biased in favor of the organizer; and the probability laws ensure that the bank in a casino, the government coffers in a lottery, or the Swiss accounts for a local Mafia (*jogo do bicho* or others) are inevitably the winners, by a hefty margin.

3. Miniatures as toys

Allow me to single out, among toys crafted or manufactured for children,[11] the following short list: dolls and doll houses;[12] toy soldiers; model trains; remote controlled vehicles (cars, airplanes); miniature cars; kites; construction sets (Erector, Lego, Meccano, *etc*.); parlor games such as Monopoly. Those all offer (and offer themselves as) a representation, as a parallel world in reduction (or microcosm), as a stereotyped object which the child can manipulate at whim and totally control.

Equally interesting, one can reflect on toys and games whose use straddles the borderline between childhood and adulthood. Monopoly belongs to this category. Let me give another few examples. Adult men, especially in Great Britain and Germany, collect model trains, and there are specialized shops in these countries catering for such railway buffs. A symbolical transposition of a battlefield is the chessboard (Vladimir Nabokov makes somewhere the illuminating comment that if Russians are so fond of chess, it is only because they were enslaved for so many centuries). Puppet shows – often with a subversive social and political function, often with a popular origin at the margins of society (but this would be an altogether separate story) – bridge the gap between role-playing by children at home and role-playing by adult actors in the theater.

All such toys stand for a complex reality which they evoke, which they allow to escape from, to conjure at the obvious cost of drastic oversimplification. Also, it is no accident that quite a few items in the above list came into fashion in the aftermath to World War I and its bloodbath: Ole Kirk Christiansen started LEGO sets in 1934;[13] Meccano production started in 1914; the Monopoly game appeared during and as a result of the Depression. Could all such games belong to an escapist *episteme* in the sense of Foucault, brought about by the mass slaughters[14] of the First World War?

Thus model houses, model cars, model airplanes, model people as represented by dolls and puppets, serve dual and complementary functions for children and for adults. They prepare the former to the real world, through establishing first familiarity with the world of toys. They allow the latter an escape, regression perhaps also, from the real world into the Lilliputian world of toys. In some rare cases too, an adult will behave as the child he was not allowed to be, because of *e.g.* recovery of a long-lost mode of perception.[15]

At this point, an obvious objection springs up: molecular models are not *mini*atures, they are *macro*tures – to use an ugly neologism – they are enlargements by many orders of magnitude over the postulated (by a form of naive realism) molecular 'objects'. The answer is equally obvious. Molecular models and miniature toys share their being representations of entities in the real world, with the attendant change in scale, also with stereotyping and severe simplifications (such as the freezing-out of time and motion in molecular models for handling). Those representations, by contrast to virtual reality, are also real objects, made of wood, plastic, metal, *etc.* They are quasi-oxymoronic illusions which one can see, touch, scratch, lick, sniff, *etc*. Their user can handle and control them at will. Such illusions belong to dummies, by contrast to mere mental images and illusions.

4. Make-believe as play

An essential dimension of play originates in a bodily gesture. The player, be he or she an infant, a child, or an adult, first shows a certain intention and then acts different from what onlookers or other players had been led to expect. Such deception, a fundamental element in warfare too, occurs in martial arts (such as judo, jiu-jitsu, aikido, *boxe française*, *etc*.), in boxing, fencing, American football, soccer, *etc.*

The underlying mental attitude is *pretending*: a general might say to himself or to his subordinates "I am pretending to move to the Northwest, in order for the enemy to follow suit with his forces; then, when I have attracted him into this particular trap, I'll try to annihilate his forces." Children often engage in pretend games: they play being parents, or a pilot, a train engineer, a car driver etc. As just mentioned, war games in a military college belong to the same class, military exercises in the field likewise. Quite a few sexual fantasies, whether acted-out or not, also belong to the same category of pretending games. Traditionally, adults indulge in pretending games at festive times, often set at a particular time in the calendar such as Carnival, when the wearing of costumes and masks is an outward representation of the role-playing.

Adults also engage in pretend games – truly mixes of play and work, the game has become to a large extent a tool, *i.e.* an adjunct with a purpose – when carrying out computer simulations, for instance of the Monte Carlo type;[16] or as when professionals, pilots for instance, use flight simulators.[17] Molecular models are thus hybrids, in-between tools and games. By handling them, the chemist acts out a set of beliefs, both individual and corporate, regarding entities in the microphysical world.

This is a game, since those entities are as elusive and inaccessible to our perception as angels or ghosts, even with the help of the most modern scientific instruments. This is a serious activity, in that these molecular models have a postulated resemblance to reality, enough as to give them operational value.

5. Models as transitional objects

The psychoanalyst Donald Woods Winnicott (1896-1971) is famous, among other influential contributions,[18] for his concept of the 'transitional object'.[19] A transitional object (TO), according to Winnicott, has the following attributes: 1. it is a material object; 2. the TO serves as a go-between the infant (at the age of four to twelve months[20]) and the world; 3. the child makes the TO an extension of himself/herself; 4. the child indeed appropriates the TO; 5. the TO is polysemic; 6. the TO is handled obsessively; 7. the TO is often soft and cuddly; 8. the TO has the function of loosening the ties to the mother and of helping the child gain his or her autonomy; 9. the TO occupies an area, mental and spatial, in-between the psyche and the physical environment, which helps the individual to acquire a symbolizing activity and prowess.

An example of a TO is Linus's security blanket which he carries around in the *Peanuts* comic strip while sucking on his thumb, a behavior emulated by an estimated 60% children in Western culture. Later, adults play with items reminiscent of TO's. Textual narratives and movies, in particular, make great use of visual allusions to such infantile relics: Sherlock Holmes's fidgeting with his pipe; Citizen Kane's Rosebud sled; or Steve McQueen's tennis ball in *The Great Escape* are such ploys. We have all seen adults fiddling likewise with a cigarette, a lighter, a matchbox, a telephone cord, *etc.* and we know how widespread such a behavior can be.

One may note, in this context, that chemists quite often adopt a formula, that of the molecule they are most concerned with, as their signature-cum-fetish: for instance, when hosted by a fellow chemist, by occasion of a seminar especially, often a request is presented to sign a guestbook. Besides the usual statements acknowledging the quality of the hospitality, the guest writes down his or her name and often accompanies it with a chemical formula. I regard such a habit as coterminous to the use of formulas as icons, first within the chemical community and then in the culture at large. Examples of the first kind are camphor, the steroid skeleton, and the porphyrin ring. Examples of the second kind are the benzene ring and the DNA double helix.

Concerning molecular models, Winnicott's profound insight translates and helps recognizing the interconnection between at least three levels: the self, the outside world or rather worlds (both macroscopic and microscopic) and this hybrid, intermediate object, the molecular model, which serves as a kind of a stick to mentally probe the physical world with. Thus, the molecular model has the eminent function of a toy: among other features, it points to an infantile regression under the cloak or umbrella of advancement of knowledge.

6. The epistemic dimension of play

Very early, construction kits were used in a school setting to kindle the interest of children in following their building instinct. When Fröbel devised the kindergarten,[21] such auxiliaries were an integral part of his program, *viz.* to make the child learn alone how to master an environment in miniature,[22] formed from wooden building blocks.[23] Indeed, Christoph Meinel has put forward the attractive (but so far totally unproven and unsupported) hypothesis of a link between the Fröbelian kindergarten and the devising by professional chemists (Kekulé, Couper, Crum Brown, Havrez and a few others) of chemical formulas and models in the heyday of structural chemistry during the 1850s and 1860s.[24] When Maria Montessori[25] devised in turn her version of the kindergarten, she was moved also by an optimistic trust in the intellectual abilities of very young children, for mathematics in particular,[26] and she devised her own set of wooden blocks and artifacts to help children acquire essential cognitive skills.[27] It remained for Jean Piaget to propose in the 1950s a genetic epistemology, relating sensorimotor development of the child and the gradual acquisition of cognitive skills.[28] Piaget has also related history of science to psychogenesis.[29]

Kits such as the Montessori set help to develop several distinct and complementary abilities, *viz.* recognition of shapes, textures and colors; assembly of modules into structures; the creativity of construction, able to not only reproduce already existing schemes but also to invent new ones; the notion of an overall shape distinct from the elementary shapes of individual modules; the construction-destruction duality (a child often takes considerable satisfaction in wrecking a carefully built contraption); the dual notion of stability-instability (a child learns how to build either a durable or a self-collapsing vertical accumulation of elements); and, related to the already mentioned destructive inclination, the experiencing of deformation *i.e.* acquiring a notion of how a given assembly can be modified and perturbed so that it will assume somewhat differing shapes.

Let us note, in particular, the realm of pleasurable feelings associated with touch and with the handling of things. The interplay between visual and tactile elements is a major component in cognition – all the more so for it being associated with sensuous and even, at times, erotic emotions.

What are the connections between a young child playfully learning the feeling and appearances of objects, on one hand, and a research scientist handling a molecular model (let us assume, for the sake of the argument and even though they are now fast disappearing, this is a concrete wood or plastic artifact)? Is there, as implied by Meinel's lovely hypothesis, another connection as well between innovative preschool or primary school teaching and innovative thinking on the part of a trained scientist?

I see three main enduring attitudes possibly fostered in childhood by playing with Fröbelian or Montessori sets of blocks. The first is autonomy: Maria Montessori wanted to endow each child with self-esteem and with enough self-assurance to carry him or her throughout life. It is not necessary to stress the importance of a critical and autonomous stance to the work by any scientist. The second is the carrying out deformations of the model, whether actually or in the mind. Children love deformation of one's face, as in grinning, grimacing or from deforming mirrors. Kindergarten self-teaching from a set of modular objects leads to alterations of constructs, as we saw. It would be an asset to any scientist to study, to foresee, and to plan organized deformations, topological for instance, of three-dimensional objects. An outstanding example is Corey's longifolene synthesis, calling for visualization of the possible link between two atomic centers formally distant, at least in a two-dimensional representation.[30]

The third potential legacy from an initiation into play with construction kits during kindergarten is in 'what if?' questions posed by scientists. At a certain age, toddlers love the showing and hiding, in quick succession, of an object, of a face or of a person. The educated, mature counterpart of such hide-and-show games is when a research scientist, behaving as an engineer and treating a system of study as a black box, says to him/herself: "what would happen if I remove this particular part? Or that other part?" Manipulation of a molecular model, especially in a playful manner, makes it easy to raise such questions – which of course is at least as important as figuring out how to answer them.

Such epistemic consequences of playing with games and models include discoveries.[31] Sports such as basketball or rugby were not born otherwise. Galileo watching during a church service, as the story goes, the pendular motion of chandeliers discovered their law of motion. Pauling, while in bed in Oxford with the flu according to witnesses such as Dorothy Crowfoot Hodgkin, played with paper models and discovered the alpha helix component of protein structure. His study of models, with which he surrounded himself during his whole life at work and at home,[32] led him to other discoveries such as the structure of rare gas hydrates.[33] Likewise, Harold Kroto associates his part in the discovery of C_{60} (also known as 'buckyball') to a soccer ball reminiscence.

Lewis Carroll can be singled out in the Victorian era for his reinjecting into literature for children the playful fun a professional scientist enjoys.[34] His writings relegate the original scientific concepts in the background; for instance, *Through the Looking Glass* arguably has to do with enantiomers and racemization, *i.e.* with the work of Louis Pasteur. In the 20th century, George Gamow at first,[35] Richard P. Feynman later on[36] displayed a kindred spirit of witty and funny science popularization.

7. Costly toys?

Like most assertions, the main thesis in this paper – chemists are wont to play with molecular models – is subject to criticism and refutation. Two of the main objections, not unrelated, are "what about the cost?" and "this is also a pedagogical tool and thus it is obviously not a toy."

Let us consider each in turn. True, molecular models at their most accurate are precision-engineered[37] and they can thus be extremely costly. This was the case indeed for CPK models as Eric Francoeur has emphasized,[38] and

Dreiding models were likewise very expensive. Regarding the latter, exquisite samples of Swiss craftsmanship, I can recall – if I may be allowed this personal note – visiting Professor E.J. Corey in his Harvard office in early 1963. Above his desk, near the ceiling he had strung a line on which a whole collection of Dreiding models was hanging. There were perhaps two or three dozens of those. They represented the structures of the complex natural products in the process of synthesis in his laboratory. I remember most vividly my shock at ogling several thousands of dollars hanging in the air. Immobilization of that sort, while rather convenient, was most expensive: a status symbol, perhaps?

The answer to this first objection is that indeed some toys, whether for children (an electric train) or for adults (a Porsche or a Jaguar) are indeed outrageously costly. In spite of their price tag, they do contribute nevertheless their bit to the self-esteem of their lucky owner.

We come to the second objection by noting that much cheaper (much less accurate too) sets are offered to students of chemistry: which relates to the topics of classroom and homework use of molecular models. The chemistry instructor is wont to complement the pictures of molecules he or she shows (movies, videos, computer output, slides, transparencies, *etc.*) or draws (blackboard, overhead projector) by building their models in front of the students. He or she can display in this manner an overall shape and significant features such as the relative rigidity of a cyclohexane ring in the chair conformation as contrasted to the flexibility of the twist boat form; or the inversion of R/S configuration attendant upon a Walden inversion; or yet the pseudorotation in a trigonal bipyramid, for say a pentacoordinated phosphorus atom.

Whereas the students follow attentively such classroom demonstrations, teachers often complain that the students' study of the subject matter does not include quite enough model building and observation, as if students had trouble switching from a passive to an active role. Why? Sometimes, the cost of models, even though it remains marginal, may be an issue. Another often-quoted reason is that many students have trouble visualizing three-dimensional geometric shapes, through lack of habit predominantly. They shy away from gaining familiarity through use of models, precisely when this would be a great help to them: try to understand! Yet another reason is the perception by students of the playful, open-ended manipulation of models. This creative feature, which allows for build-up of all sorts of structures, runs afoul of the implicit teacher-student contract which specifies and circumscribes the exact subject matter to be learned, memorized and regurgitated at examination time.

Recently, historians of science have often commented about the didactic origin of various forms of representation of nature and of matter, such as chemical formulas and three-dimensional models. This is a worthwhile observation. However, regarding models, the 'show-and-tell' dimension remains secondary, at least to this practitioner, to the inspection of models in the half-serious, half-playful mode of the scientist tinkering with such a toy in his/her search for a significant problem to address and solve. We close up now with consideration of this all-important mute dialog between the scientist and the model.

8. *Homo chimicus ludens*

The chemist looks at his model. Notice how this last sentence parallels this other sentence: the artist looks at his model. There are similarities and differences. Similarities include the intensity of the look, the confrontation between the viewing and the imagining, *i.e.* between the object sitting out there being looked at and an image in the mind. There is a more distant analogy too: the chemical model, just like a work of art made after a model, can be unfinished and be still in a somewhat inchoate state. A difference is that, while often a model for a painting or a sculpture is a real person or an animate part of nature, the model the chemist views and ponders is an inanimate assembly.

Another analogy springs to mind. The chemist observes his (or her) model in like manner as Daedalus inspecting a *daidalon*, a device of his design and make. This is the attitude analogous to that of an architect inspecting a miniature model of a construction, or likewise of an engineer examining a dummy reproduction of a bridge, a ship or an aircraft.

The chemist studies the model with full awareness of the two complementary modes of perception, touch and sight. The molecular model bridges them, and this is an essential feature. The scientist handles the model, feels his way around it, thus anthrophormizing it. He or she scrutinizes the model, looks at the relationships between the parts. A phrase such as 'non-bonded interactions' is unthinkable outside of the practice of model building and model viewing. The scientist pays special, careful attention to potential complementarities of shapes, since he/she knows how important such congruences of the lock-and-key type (Emil Fischer)[39] are *inter alia* to biological activity. *Homo chimicus* thus links across the ages with *Homo sapiens* (or *Homo sapiens sapiens*) when in the Neolithic (if not earlier) tools were being carefully manufactured: scrapers, arrowheads, *etc.*

To sum up: to the professional chemist, molecular models are as much toys as they are tools.[40]

Acknowledgments

I am most grateful to Professor Roald Hoffmann for his reading of this paper at the proof stage and for some excellent suggestions. His personal calling card, for not showing a molecular structure proper, nevertheless displays his trademark, in the manner of one of the molecular orbitals for methane inscribed within a cube; which is as good an example as any for one of the points made in this paper.

Notes

1 Hoffmann, R. and Laszlo, P.: 1989, 'Representation in Chemistry', *Diogenes*, **147**, 23-50; Hoffmann, R. and Laszlo, P.: 1991, 'Representation in Chemistry', *Angewandte Chemie International Edition in English*, **30**, 1-16.

2 Laszlo, P. and Hoffmann, R.: 2000, 'Ferrocene Story', *Angewandte Chemie International Edition in English*, **39**, 123-124.

3 Hoffmann, R. and Laszlo, P.: 1998, 'The Say of Things', *Social Research*, **65**, 653-693.

4 A colleague has taken issue with a remark of mine on the limitations of the sociological approach to the history of science, for which I gave concrete examples. He denigrates, instead of considering the point made and attempting to answer it constructively: Brakel, J. v.: 1999, 'Book review of The Autonomy of Chemistry, ed. by P. Janich and N. Psarros', *HYLE*, **5**, 166-168.

5 Berne, E.: 1964, *Games People Play. The Psychology of Human Relationships*, Grove Press, New York.

6 Huizinga, J.: 1951, *Homo ludens. Essai sur la fonction sociale du jeu*, Gallimard, Paris.

7 Caillois, R.: 1967, *Les jeux et les hommes*, Gallimard, Paris.

8 With a notable exception, that of automata such as Vaucanson's, see Cardy, M.: 1986, 'Technology as play: The case of Vaucanson', *Studies on Voltaire and the Eighteenth Century*, **241**, 109-123.

9 Derrida, J.: 1967, 'La Structure, le signe et le jeu', in: *L'Ecriture et la différence*, Le Seuil, Paris.

10 Borel, E.: 1937, 'Eloge du jeu', *Mercure de France*, **275**, 290-301.

11 Brown, K. D.: 1990, 'The Children's Toy Industry in Nineteenth-Century Britain', *Business History*, **32**, 180-197; Burton, A.: 1997, 'Design History and the History of Toys: Defining a Discipline for the Bethnal Green Museum of Childhood', *Journal of Design History*, **10**, 1-21.

12 Formanek-Brunell, M.: 1993, *Made to Play House: Dolls and the Commercialization of American Girlhood, 1830-1930*, Yale University Press, New Haven.

13 LEGO: 1994, *LEGO Facts & Figures*, 18th, LEGO Group, DK-7190 Billund, Denmark.

14 Céline, L.-F.: 1932, *Voyage au bout de la nuit*, Denoël et Steele, Paris.

[15] Sacks, O.: 1995, 'To See and Not See', in: *An Anthropologist on Mars*, ed. by A.A. Knopf, New York.

[16] Replete with hidden assumptions so that some authors will triumphantly point to the superb agreement of such calculations with observations when they had loaded the dice to the extent that their conclusions merely mirror their starting axioms: see for instance Delville, A.: 1994, 'Monte Carlo simulations of the mechanical properties of charged colloids', *Langmuir*, **10**, 395-402. See also for a critical and insightful description of Monte-Carlo methods, Galison, P.L.: 1997, *Image and Logic: The Material Culture of Microphysics*, University of Chicago Press, Chicago.

[17] Watkins, C. and Marenka, S.: 1994, *Taking Flight: History, Fundamentals and Applications of Flight Simulation*, N&T Books, New York; Shater, M.F.: 1993, 'In-Flight Simulation at the NASA Dryden Flight Research Facility', *AAHS Journal*, **38**, 260-277.

[18] Jacobs, M.: 1995, *D.W. Winnicott*, Sage, Thousand Oaks, CA; Kahr, B.: 1996, *D.W. Winnicott: A biographical portrait*, International Universities Press, Madison CT. Crystal Woodward, in her biography (unpublished) of her father Robert B. Woodward, a Nobel laureate and a genius of 20th century chemistry, makes the same point: a molecular model fulfills, to the professional chemist, a function closely similar to Winnicott's transitional object.

[19] Winnicott, D.W.W.: 1942, 'Pourquoi les enfants jouent-ils?', in: *L'enfant et le monde extérieur*, Payot, 1957, Paris, pp. 123-128; Winnicott, D.W.W.: 1951-1953, 'Objets transitionnels et phénomènes transitionnels', in: *De la pédiatrie à la psychanalyse*, Payot, Paris.

[20] Other authors place the peaking of the attachment to a transitional object between 18 and 30 months.

[21] Brosterman, N.: 1997, *Inventing Kindergarten*, New York.

[22] Fröbel, F.: 1851, 'Anleitung zum rechten Gebrauche der dritten Gabe', in: *Friedrich Fröbel, Ausgewählte Schriften*, ed. by H. Heiland, Düsseldorf, München 1974, pp.121-161.

[23] Noschka, A. and Knerr, G.: 1986, *Bauklötze staunen: Zweihundert Jahre Geschichte der Baukästen*, München.

[24] Meinel, C.: 1998, 'Modelling a Visual Language for Chemistry, 1860-1875' (lecture presented at the Wellcome Institute for the History of Medicine and the Science Museum, London 1998).

[25] Babini, V.P.: 1995, *Intersezioni*, *A15*, 171-174; Pollard, M.: 1990, *Maria Montessori*, Gareth Stevens Children's Books, Milwaukee WI.

[26] Jarrell, R.H.: 1998, 'Play and Its Influence on the Development of Young Children's Mathematical Thinking', in: *Play From Birth to Twelve and Beyond. Contexts, Perspectives and Meanings*, ed. by D.P. Fromberg and D. Bergen, Garland Publishing, New York.

[27] Fisher, D. C.: 1965, *Montessori For Parents*, New Editions / Robert Bentley, Cambridge, MA.

[28] See *inter alia*: Piaget, J.: 1952, *The child's conception of number*, Humanities Press, New York; François, F.: 1978, *La psychologie de Jean Piaget et l'analyse de l'acquisition du langage par l'enfant*, Université Louis Pasteur, Strasbourg; Bringuier, J.-C.: 1977, *Conversations libres avec Jean Piaget*, Robert Laffont, Paris; Good, R.; Mellon, E.K. and Kromhout, R.A.: 1978, 'The Work of Jean Piaget', *Journal of Chemical Education*, **55**, 688-693.

[29] Piaget, J.: 1973, *To understand is to invent*, Grossman, New York; Piaget, J. and Garcia, R.: 1983, *Psychogenèse et histoire des sciences*, Flammarion, Paris; Messerly, J.G. : 1996,'Psychogenesis and the history of science: Piaget and the problem of scientific change', *Modern Schoolman*, **73**, 295-307.

[30] Corey, E.J.; Ohno, M.; Vatakencherry, P.A. and Mitra, R. B.: 1961, *Journal of the American Chemical Society*, **83**, 1251.

[31] Laszlo, P.: 1999, *La découverte scientifique*, Presses Universitaires de France, Paris.

[32] Nye, M. J.: 'Paper Tools and Molecular Archictecture in the Chemistry of Linus Pauling', in: *Proceedings of the conference on Paper Tools and Traditions of Representation in the History of Chemistry, Max Planck Institute for the History of Science, Berlin, 2-4 December 1999*, ed. by U. Klein, forthcoming.

[33] Catchpool, J.F.: 1968, 'The Pauling Theory of General Anesthesia', in: *Structural Chemistry and Molecular Biology*, ed. by A. Rich and N. Davidson, Freeman, San Francisco, pp. 343-355.

[34] Gardner, M.: 1996, *The universe in a handkerchief: Lewis Carroll's mathematical recreations, games, puzzles, and word plays*, Copernicus, New York.

[35] Gamow, G., Stannard, R. and Edwards, M.: 1999, *The New World of Mr. Tompkins: George Gamow's Classic Mr. Tompkins in Paperback*, Cambridge University Press, Cambridge.

[36] Feynman, R. P.: 1985, *Surely you're joking Mr. Feynman*, Bantam, New York.

[37] Usually, the scientist relies on a model-maker, often from the machine shop. One wishes to know more about such interaction, it is quite important. See for some closely related examples Hughes, T.P.: 1988, 'Model Builders and Instrument Makers', *Science in Context*, **2**, 59-75.

[38] Francoeur, E.: 1997, 'The Forgotten Tool: The Design and Use of Molecular Models', *Social Studies of Science*, **27**, 7-40.

[39] André-Marie Ampère in his 1814 paper on representative shapes of molecules, a key paper in the history of chemistry, was prophetic also in his insistence on the importance of congruent shapes for molecular assembly: Ampère, A.-M.: 1814, 'Lettre de M. Ampère à M. le comte Berthollet, sur la détermination des proportions dans lesquelles les corps se combinent d'après le nombre et les dispositions respectives des molecules dont leurs parties intégrantes sont composées', *Annales de Chimie et de Physique*, **XC**, 43.

[40] "A model is something to be admired or emulated, a pattern, a case in point, a type, a prototype, a specimen, a mock-up, a mathematical description – almost anything from a naked blonde to a quadratic equation – and may bear to what it models almost any relation of symbolization." N. Goodman, *Languages of Art. An Approach to a Theory of Symbols*, Hackett Publishing Co., Indianapolis, 1976, p. 171.

Pierre Laszlo:
Institut de chimie B6, Université de Liège au Sart-Tilman,
B-4000 Liège, Belgium; Pierre.Laszlo@ulg.ac.be

and. Playing with Molecular Models 93. Dreiding models were likewise very expensive. Regarding the latter, exquisite. samples of Swiss craftsmanship, I can recall â€“ if I may be allowed this person-. al note â€“ visiting Professor E.J. Corey in his Harvard office in early 1963. Above his desk, near the ceiling he had strung a line on which a whole collec-. tion of Dreiding models was hanging.Â Playing with Molecular Models 95. Acknowledgments. I am most grateful to Professor Roald Hoffmann for his reading of this paper. at the proof stage and for some excellent suggestions. His personal calling. card, for not showing a molecular structure proper, nevertheless displays his. trademark, in the manner of one of the molecular orbitals for methane in Biomolecular Modeling: Goals, Problems, Perspectives, W. F. van Gunsteren, D. Bakowies, R. Baron, I. Chandrasekhar, M. Christen, X. Daura, P. Gee, D. P. Geerke, A. Glattli, P. H. Hunenberger, M. A. Kastenholz, Lecture 21 (Apr 2): Tutorial & Introduction to AutoDock [PDF]. C. Oostenbrink, M. Schenk, D. Trzesniak, N. F. A. van der Vegt and H. B. Yu, Angewandte Chemie International Edition, 45, 4064-4092 (2006) [PDF].Â Computational Quantum Mechanics & Advanced ab Initio Methods, Chapters 2 & 3 from Molecular Modeling, 2nd Edition by A. R. Leach [PDF]. Derivation of the Hartree-Fock Equation, Appendix 7 from Quantum Chemistry, 3rd Edition by J. P. Lowe and K. A. Peterson [PDF]. Approximate Molecular Orbital Methods. molecular-modeling molecular-analysis md-data-analysis. Updated Jul 20, 2020.Â SwarmCG: Automatic Parametrization of Bonded Terms in Coarse-Grained Models of Simple to Complex Molecules via Fuzzy Self-Tuning Particle Swarm Optimization. optimization molecular-dynamics optimization-tools gromacs coarse-grained coarse-graining molecular-modeling. Updated Aug 17, 2020.