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THE ROLE OF ANALOG MODELS IN THE UNDERSTANDING OF THE NATURE OF MODELS IN CHEMISTRY

1. MODELS AND MODELLING IN CHEMISTRY

Models play a vital role in chemistry because they can serve a wide range of functions. They can represent complex phenomena, make abstractions more readily visualizable, enable predictions to be made, provide the basis for the interpretation of experimental results, and, most importantly, enable explanations to be devised (Francoeur, 1997; Gilbert, Boulter, Rutherford, 1998; Tomasi, 1988; Rouse & Morris, 1986). These functions are made possible by the scope of their attributes. They can be made to concentrate on different aspects of a phenomenon, being produced for different purposes. The phenomenon represented can be an object (e.g., a distillation apparatus), an event (e.g., the collection of a required distillate), a process (e.g., the progressive separation of types of molecules), or ideas (e.g., the distribution of molecular velocities in a mixture). They are readily adapted or replaced as scientific circumstances require. Lastly, they enable discussion between scientists to take place readily.

Chemistry is essentially a science of abstractions. As a consequence of this, chemists must represent the phenomena they observe (at the macroscopic level), the ideas with which they try to explain such phenomena (at the sub-microscopic level), and a shorthand summary of what is going on (at the symbolic level) (Johnstone, 1993). At the macro-level and sub-microscopic level, models are used to facilitate the visualization of what is happening. In doing so, all the characteristics and roles of models above mentioned permeate chemistry. Chemical models may be static or dynamic. They may be expressed in concrete (three-dimensional), visual (two-dimensional or pseudo-three-dimensional: computerised), and/or verbal modes of representation. At the symbolic level, mathematical equations, or the special language of chemical equations, are used. Moreover, chemists are able to transform models from one mode of representation into equivalent representations into other

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modes (Kozma & Russel, 1997). The transformation of models in this way focuses attention on different aspects of them for example, their relationship to quantification, their behaviour through time, and the reproducibility of their behaviour (Boulter & Buckley, 2000). Thus chemical knowledge is produced and communicated with the use of several models, which evolve and are changed as the field of enquiry advances.

Chemical ideas seem to have been visually, verbally, or mathematically, modelled ever since they were first produced. However, the production of the first concrete models for atoms by John Dalton at the beginning of the nineteenth century was as a landmark in the way that models have contributed to the development of chemical knowledge. The visualization of cause and effect became possible for the first time. Following him, leading scientists, such as Kekulé, Van't Hoff, Pauling, Watson and Crick, have made increasing use of concrete models to present visually, develop and discuss their ideas about molecular structures. This enabled them to predict the behaviour of the substances they were modelling and to speculate about the spatial arrangements of atoms and functional groups in their structures (Francoeur, 2000). Molecular models thus became obligatory tools in the study of the stereochemistry, properties, and reactivity, of substances which, in turn, corroborated atomic theory (Francoeur, 1997).

In recent years, computational models and modelling have become comprehensively established in chemical research. Two factors seem to have contributed to this. First, the study of the dynamics of chemical reactions – the mechanisms by which they occur – required the production of more complex models. Static and rigid molecular models, as well as their two-dimension representations (formulas and equations – even when curly arrows are used), were shown to have a limited utility for this purpose. Second, the introduction of quantum mechanics provided chemistry with a new research programme (in Lakatosian terms) which allowed chemists to go beyond qualitative descriptions and even to predict the properties of materials which have not yet been synthesised (Erduran, 2001; Mainzer, 1999). The ability to access large amounts of data on a variety of aspects of chemical substances and to present data at a number of different representational levels (Ealy, 1999) has made computational modelling an essential tool for investigating known and new substances and their transformations. The approach is also vital in probing the properties and uses of new materials – undoubtedly one of the currently most important areas of chemical research.

2. MODELS AND MODELLING IN CHEMISTRY TEACHING

In order for students at all educational levels to develop a comprehensive understanding of chemistry they should come to address all of Hodson's (1992) list of general purposes for science education. They should: (i) come to know the major chemical models (including their scope and limitations); (ii) have an adequate view of the nature of models and be able to appreciate the role of models in the accreditation and dissemination of the products of chemical enquiry; and (iii) be able to create, express and test their own models. Moreover, modelling activities may also provide especially valuable opportunities for teachers to monitor students" progress in changing from their initial mental models to an understanding of established models (Duit & Glynn, 1996). Therefore, the key to the achievement of a comprehensive understanding of chemistry is the act of modelling. It is from building and manipulating a model that we can learn more than simply by looking at a representation of it (Morrison & Morgan, 1999).

An analysis of historical examples of the ways in which modelling resulted in the development of important scientific knowledge shows that this is a dynamic and complex process. Each scientist's reasoning is influenced by both the purpose for a particular model and the whole context in which it is produced. On account of this, there are no general rules for model construction (Morrison & Morgan, 1999). However, in order to guide science teachers in the introduction of modelling activities into their classes, we developed a general framework for the modelling process (Justi & Gilbert, 2002). This is a logical idealisation of what takes place but, in the present absence of classroom-based case studies, cannot be seen as a representation of what actually takes place. This framework is presented in Figure 1 and explained next. In an educational situation, the *purpose* for which a model is to be built must be clear to the students. By having such a purpose in mind, they may focus their attention on the entities to be modelled. These may arise from simultaneous *observations of* and *experience with* the phenomenon. They may be direct or indirect, qualitative or quantitative, depending on both the purpose of the activity and the context in which it takes place. At the same time, students may think about possible *sources* from which the model might be derived. As a result of such a process, an initial mental model would be produced and expressed in a suitable mode of representation: material, visual, verbal, mathematical, gestural. This process of expression may be seen as cyclically developmental in respect of the mental model, with the act of expression leading to a modification of it.

Having produced a model, the next phase would involve testing it. This may start from an exploration of the model's implications through *thought experimentation* conducted in the mind. As Reiner and Gilbert (2000) have commented, it is likely that scientists always mentally rehearse the design and conduct of empirical experimentation. It is only when the outcomes of this mental activity seem successful that actual empirical testing takes place, where this is possible. If the model fails to produce predictions that are confirmed in the thought experimental testing phase, then an attempt would have to be made to modify it and to re-enter the cycle. However, if it passes the thought experimental phase, it would go on the *empirical testing* phase. This would entail the design and conduct of practical work, followed by the collection and analysis of data, and finally by the evaluation of the results produced against the model. If the model fails at this stage, an attempt would have to be made to modify it and subsequently to re-enter the cycle. However, if it passes the empirical testing phase, the student would feel confident that the purpose for which it was constructed has been *fulfilled*.

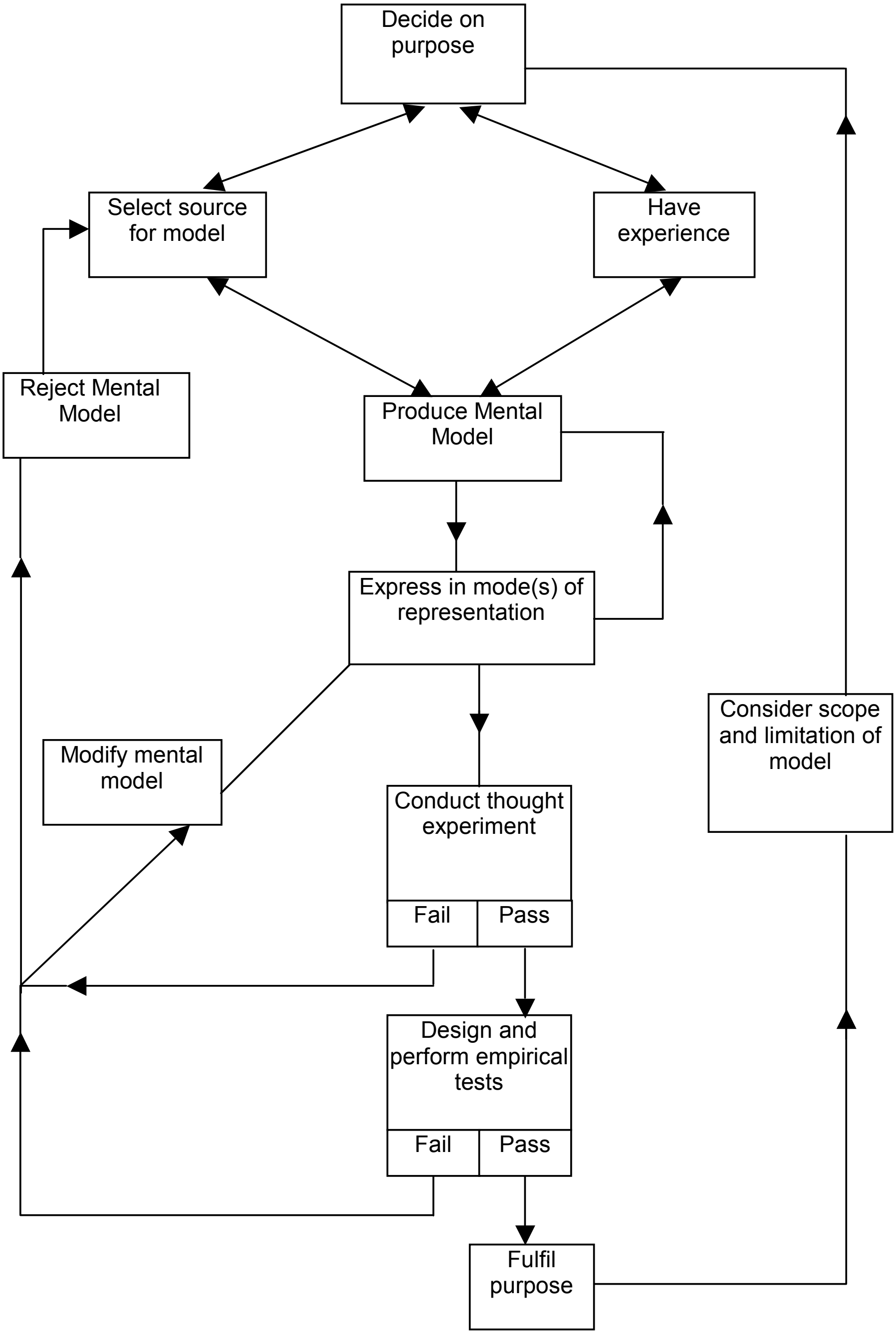


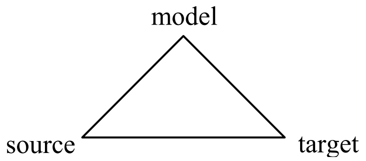
Figure 1. A "model of modelling" framework

This would be followed by a phase in which an attempt would be made to persuade others (peers and the teacher) of its value. During this process of advocacy, the *scope and limitations* of the model would become apparent, leading to a reconsideration of the earliest elements in the model-production cycle. If the sub-cycles of model modification and thought and/or empirical testing were repeatedly unsuccessful, then the model would have to be rejected. This would lead to a radical reconsideration of the earliest elements in the model-production cycle. The introduction of this framework to students implies both the development and use of several skills and knowledge. It should result in the achievement of the comprehensive understanding of chemistry previously discussed. This introduction could be conducted from different methodological perspectives in different educational contexts. We do not believe that the framework itself should be taught to students prior to the proposition of a modelling activity. The risk that they merely learn the framework rather than be able to use it in some way is too great. A much better use for the framework is to help teachers think about their classroom practices in general and how to change them so they become *generally* more model-based and modelling-oriented.

3. ANALOGIES AND MODELLING

An analogy, as emphasised in other chapters of this book, expresses a relation of equivalence or likeness. This means that when we say ‘A’ is analogous with ‘B’, we are saying that there are some aspects of ‘A’ that *are like* aspects of ‘B’. Analogies are employed throughout the realm of language use because they are powerful tools in the understanding of new domains. This is so because, when an analogy involves a target that is unknown and a source that is known for someone, this is followed by the establishment of new relationships between them.

In one of his best-known papers, Duit asserted that: “It is the analogy relation that makes a model a model” (Duit, 1991, p.651). Such an assertion was made from the recognition that models, as analogies, “have to do with the structural mapping of different domains” (Duit, 1991, p.651). According to this view, we may represent the process of creation of a model through the diagram:



In this representation:

- “Target” is the aspect of reality that is being modelled. It may be an object, an event, a process or an idea.
- “Source” is some more familiar entity that is used to represent the target through the production of an analogy.

- “Model” is the result of this representation.

Historically, the building of analog models was very important in both the development and communication of scientific knowledge. The more detailed examples found in the literature come from physics. Nersessian (1999), for instance, after emphasising that analogical reasoning is a kind of modelling activity, explains how Maxwell constructed the visual model of “electromagnetic field” by the building of an analog model and from several tests on it to improve its scope of representation and capacity for generating predictions. Nersessian also comments about Maxwell’s use of his model in communicating the knowledge he created and in trying to convince other scientists of its potential.

In chemistry there are also examples in which the building of an analogy had a pivotal role in the modelling process that resulted in the production of new knowledge. In identifying the historical models in the development of the field of chemical kinetics (Justi, 1997, Justi & Gilbert, 1999), we realised how the use of different analogies for the key concept of chemical reaction was vital in the evolution of explanations of “rate of reaction”. Some of them are presented next.

In the seventeenth and eighteenth centuries, the gradual development of corpuscular views of matter meant that the concept of “affinity”, introduced by the Greek philosophers from the attribution of the human qualities of love and hate to the elements, changed in character. Boyle, for instance, built a mechanical analogy according to which “affinity” was a result of corpuscles having appropriate shapes which permitted them to adhere together and which did not result from an attraction force. On the other hand, Newton, from an analogy with his studies in physics, thought “affinity” was a sort of force by which bodies tended toward one another, whatsoever was the cause (Duncan, 1996; Levere, 1971). This was the first time that the origin of a “force” that brings about a chemical reaction was seen to be related to the characteristics of particles as such or as originated from them. By being somewhat more precise about the forces operating between reacting substances, a model for chemical kinetics facilitated predictions about the likelihood and rate of a reaction. Within this model, the rate of the transformation was related to the different degrees of affinity between the particles and depended on its readiness to occur (Justi & Gilbert, 1999).

At the beginning of the last century, another powerful analogy was proposed for chemical reactions. Assuming the kinetic theory of gases, Trautz and Lewis, working separately, proposed that the behaviour of molecules was analogous to that of hard spheres. For them, the collision of the molecules produced a reaction only if it occurred with both sufficient energy and at an appropriate orientation such that specific bonds were broken and made. Then, from this overall view of how collisions occur, they also related the “frequency factor” – previously defined by Arrhenius – to the frequency of collisions between reacting molecules and calculated the magnitudes of frequency factors (Laidler & King, 1983). These examples show how the choice of a given source for an analogy led to the development of specific models for “reaction rate”.

However, the analogies were not the only origin of such models. According to the framework presented in Figure 1, a mental model is produced as a result of integration between three steps that sometimes occur simultaneously: “decide on purpose", "have experience" and "select source for model". From the chemical kinetics perspective, we may say that the purpose in all the cases was the same: to explain reaction rate. But the selection of the analogies, as well as the way in which analog relationships were established between the source and the target, was determined by what could be empirically observed at the time.

This is the stage in the modelling process (Figure 1) where analogies are most evident. But they can also exert roles at other stages of this process. The next stages – "produce a mental model" and "express it in any mode of representation" – may also involve analogical reasoning. For example, in 1850, Wilhelmy studied the rate of inversion of sucrose by using a polarimeter to follow the decomposition of saccharose into two monosaccharides in the presence of an acid. The polarimeter did not disturb the conditions of the reacting system and he observed that the instantaneous rate of change of the sugar concentration was proportional to the concentration of both the reactants. Thus, from an analogy to the mathematical and physical theory of heat – that he had studied before – he proposed a mathematical differential equation to express and explain his ideas. This was the first time that the rate of a reaction was treated quantitatively (Laidler, 1995).

Finally, the stage of testing a model and its consequences – leading to either the modification or rejection of the model or to the consideration of its scope and limitations – can also make the role of analogies and analogical reasoning evident. As was said before, in the seventeenth and eighteenth centuries, two main analogical models for "affinity" were accepted. According to one of them, "affinity" was a result of corpuscles having appropriate shapes which permitted them to adhere together and which did not result from an attraction force. However, it also was at that time that empirical experimentation started to become essential for the acceptance of chemical ideas. It was exactly due to such an empiricist tradition that this analogical model for affinity decreased in importance. Aspects such as shapes, sizes, and mechanisms of particle adhesion, could not be tested experimentally (Duncan, 1996). Thus, as the main elements of the source of the analogy could not be transferred to the target in the testing phase of the model, such an analogical model could not fulfil its purpose and was soon rejected by the scientists working in that field. On the other hand, one of the followers of the Newton's analogical model – "affinity" was a sort of force by which bodies tended toward one another – Wenzel proposed an extension of this analogy that was able to increase the acceptability of the model. This was done not only by successfully testing the analog relationship itself but also by producing new knowledge from it. According to him, the magnitude of a force in mechanics was measured by its influence upon the motion of a body. If affinity between particles was a sort of force, it should be possible to determine the magnitude of this force – chemical affinity – by measuring its influence in the rate of the occurrence of reactions (Mellor, 1904). By empirically studying the rate of dissolution of a metal by an acid, he found out that such a rate depended not only upon the nature of the metal, but also upon the concentration of the acid. Therefore, he proposed that "a chemical action is proportional to the amount of substances taking part in the reaction".

In sum, the analysis of all the examples presented above corroborates the idea that analogies are very important, and may even be essential, in modelling chemical entities. As the source of the model is changed, so does the nature of the target that can be successfully explained. The "hard spheres" analogy enabled distributions of molecular energy to be represented and hence the availability of energy for bond breaking to be conceptualised. The "mathematical and physical theory of heat" analogy enabled differential equations to be used in constructing rate equations. The "chemical affinity as a force" analogy enabled the amount of substances involved in reactions to be represented.

4. ANALOGIES AND MODELLING IN CHEMISTRY TEACHING

The roles of modelling in chemistry and of analogies in modelling suggest a distinctive place for analogies in chemistry teaching and learning: their invaluable contribution to the understanding of the nature of models and modelling. Such a perspective may be analysed at different levels.

As previously emphasised, visualizable chemical knowledge at the macroscopic and sub-microscopic levels is based on models. This has been recognised as one of the factors that make understanding chemistry difficult for students at all educational levels (Gabel, 1999; Johnstone, 1993; Treagust & Chittleborough, 2001; Wu, Krajcik, & Soloway, 2001). This is because the major chemical explanations are derived from the use of models of sub-microscopic – thus abstract – entities. Moreover, such researchers assert that difficulties in chemistry learning do not only arise from the existence of these different levels, or even from the inherently abstract characteristic of chemical explanations, but also from the disconnected way in which they are often presented to students. Therefore, students are not able to integrate the two levels and to construct a comprehensive understanding of chemistry.

According to Gabel (1999), one of the ways to help students to establish relationships between these different levels is through work in the laboratory. However, this would not be so in the case of traditional practical work – that which can be characterised as the following of a recipe – the purpose of which is to illustrate something already known. Following Johnstone, Gabel asserts that "one reason why students find chemistry difficult is that in the laboratory, they make observations at the macroscopic level, but instructors expect them to interpret their findings at the microscopic level (Gabel, 1999, p.549). Therefore, what seems missing in the process is the provision for students of opportunities to *visualise* the sub-microscopic level in such a way that they can establish relevant relationships with the macroscopic level.

From both our belief in the central role of modelling in the development of scientific knowledge and the importance of analogies in the modelling process, we suggest that such visualization can only be achieved by the involvement of students in producing and using analog models. The production and/or understanding of a model based on an analogy with something that is familiar to students should result in a way to visualise the sub-microscopic level. This can then be the basis of an understanding of its role in explaining the given phenomenon at the macroscopic level. Such an approach is the main reason for the use of analog models in both science and science teaching.

In chemistry teaching, the analog systems most frequently used for such a purpose are molecular models, especially ball-and-stick models. In a ball-and-stick molecular model, atoms or ions are assumed to be hard spheres and the main bonds between them are represented by "sticks" in a way that the final model has a structure that is similar to the one that is believed to occur in the real substance. By building or using molecular models, students can visualise such a structure, thus becoming able to understand the properties and behaviour of substances (macroscopic aspects, those capable of being observed in nature or in practical work) that are explained from particularities of the structure of the substances. Moreover, by changing the analog model – for instance, by using space-filling instead of ball-and-stick models – the teacher can make clear to the students how the choice of the analogy influences the model produced and hence its explanatory power.

The use of analog models in teaching can also help students to understand the second stage of the modelling process – where mental models are produced and expressed in different modes of representation. In teaching how chemical reactions occur, the model proposed by Trautz and Lewis can be expressed in a range of modes of representation. This model proposed that collisions between molecules cause reactions if they occur with sufficient energy and with an appropriate orientation such that the necessary bonds are broken and made. The teacher can, for instance, draw particles showing all the substances involved in the reaction, both reactants and products. This is a very common way to express the model but very frequently results in students' misunderstandings. These are due to the absence in the representation of essential aspects of the model, mainly the movement of the particles and the presence of more than a few particles of each reactant. On the other hand, the teacher can use a computer simulation to express the analog models. Here the atoms that constitute each substance are represented as spheres of different colours and sizes, binding to each other to form many particles of each substance. Such sets of spheres move within the simulation in a way analogous to how it is believed that particles of given substances move at a specific temperature. Bonds are broken and made when the necessary conditions are satisfied. When a teacher presents both forms of the model to the students, it is possible to discuss the notion that the choice of mode of representation is important in expressing any one model. Where such a discussion follows an activity in which students build their own models for a given phenomenon, the teacher could also lead them to appreciate how their choice of a given mode of representation could have impacted on the process of the production of the model itself.

The testing of analog models can also help students to understand both specific aspects of the scientific model that they are learning and the importance of testing models as such. In addressing the properties of gaseous substances, teachers turn to the sub-microscopic level and deal with the behaviour of gaseous particles. In so doing, some of them introduce a dynamic analog model (in a gestural mode of representation) in which the students themselves take on the role of particles and move in a defined area at a given rate. By decreasing the area in which they walk, students can "feel" what happens when the volume of a gas is decreased. In another test, the area where they move is not changed, but they start running instead of walking. In this case, they can "feel" what happens in a gaseous system when the temperature is increased. Several other tests can be made by using this analog model. In all of them students become able to understand different aspects of the particulate model of matter. Moreover, students can also test their own ideas about such a model, a process that may result in either changing some previous ideas or refining the model. By using this analog model in this way and by discussing such use, students can also understand the nature of the stage of "empirically testing a model" and its possible consequences.

It is of pivotal importance that the scope and limitations of an analogy are discussed with students at the stage of the modelling process that is focused on its use. They must understand that only some of the elements of the analog model are transferable to the target. For example, ball-and-stick models imply that atoms are solid, that they are not in "contact", and that bonds have no significant width. Space-filling models do not clearly represent bond angles. From the modelling perspective, this discussion is of pivotal importance since it may help students to understand the essence of the nature of models: that they are partial representations.

5. ANALOG MODELS IN CHEMISTRY TEACHING – IMPLICATIONS FOR TEACHERS

An emphasis not only on a chemical phenomenon under discussion, but also on the nature of all the elements (target, analogy and model) and the processes (analogical reasoning and modelling) involved in representing it can, as we have argued, contribute to an improvement in chemistry teaching and learning in a variety of ways.

In addition to learning how to go about producing a model, students would also come to understand what a model is and what it can do and cannot do. This would provide an invaluable window into that most exotic of topics: the philosophy of chemistry. For the chemistry teacher and student, the gains would be both more immediate and very powerful: to be able to fluently link the macroscopic and sub-microscopic realms of chemical representation.

How to go about the introduction and sustained use of modelling activities at the classroom and laboratory level will present considerable challenges to teachers. The development of case studies of how this was done in history seems an obvious way forward. The fields of enquiry into "acid/base chemistry", "chemical periodicity", "chemical bonding" are sufficiently well documented to enable them to be used for this purpose. However, there will be no substitute for students actually modelling for themselves. This will entail the identification of chemical phenomena that are capable of effective address by students at a given level of overall knowledge and understanding of chemistry. It is especially important that they have "ownership" of the problem addressed, for it is only if they are committed to a task that they will exercise their full analogical imagination. Students will need adequately large blocks of time in which to tackle any chosen task. They will need access both to laboratories and to the full range of tools with which all the modes of representation can be expressed if they are to succeed. Most importantly of all, teachers will have to suspend the "show and tell" approach in favour of "discuss and guide". The rewards for such effort should be considerable.

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