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On the Nature of Theoretical Research: Comments on Trinajstić's Paper

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In a recent paper[1] Trinajstić discussed the relationship between theoretical and experimental research. The present paper is an attempt to more thoroughly discuss several problems raised by Trinajstić; namely, what is knowledge, the definition of science and the process of theoretical research.

In a recent essay, which appeared in this Journal,[1] Trinajstić addressed – among other important questions – the relationship between theoretical and experimental research. Trinajstić concluded that theoretical research is a hierarchical composite of various stages, where the stages (such as identification of the problem, creation of a computer program, *etc.*) are all necessary ingredients of what he calls theoretical research. The other issues discussed by Trinajstić – and which I would like to comment – include: knowledge, definition of science, and the value of a theoretical framework. I think that the present list of problems raised by Trinajstić is interesting enough for scientists doing research in chemistry, and my intention is not to criticize Trinajstić's position, but to discuss these concepts more thoroughly. In particular, my arguments are intended to show that, although research in general – and theoretical research in particular – may encompass all stages suggested by Trinajstić, the stages themselves are not necessary to define the notion of »theoretical research«. In other words, the stages are criterial rather than necessary connections.

The structure of this paper is the following: first, I will review the definition of the concepts »knowledge« and »science« and then the relationship between experiments and theory. After this, the »value« of a theoretical framework will be discussed briefly.

The notion of »knowledge« is most fundamental in science but also in other realms of mental activity. Nevertheless, it is surprising to learn that many people would confuse this concept with other concepts, such as belief, or in Trinajstić's case – with the aesthetic experience that is conveyed to us by a work of art. The philosophical discipline that investigates knowledge is known as epistemology. Analytical philosophy maintains that there are three constituents, all of which together make up knowledge. The sentence »*X* knows that *p*«, where *X* denotes a name variable and *p* denotes a proposition, is true if; 1. *X* believes that *p*, 2. *p* is true and 3. *X* is justified to state the truth of *p*. Note that, instead of defining the concept of »knowledge«, it is easier to specify in which cases we are justified to claim that *X* knows something. The concepts of belief and justification need further explanation: *X* believes that *p* iff (»iff« is equivalent to »if and only if«) *X* thinks that *p* is true. *X* is justified to state that *p*, iff *X* has sufficient evidence supporting his claim that *p*. The concept of truth will be briefly discussed later. All three conditions are necessary and together they are sufficient to state that »*X* knows that *p*«. *X* cannot know that *p* if he or she does not believe that *p*, *X* cannot know that *p* if *p* is not true, and *X* cannot know that *p* if *X* has not some evidence confirming that *p* is true.

What we understand under the notion of »truth« is a difficult problem. Most scientists accept (at least tacitly) the coherence theory of truth. According to this theory, a proposition *p* is true iff *p* does not contradict other theories already accepted. But this criterion is not sufficient, and it may turn out that *p* is not in accordance with accepted theories, yet *p* is true and accepted theories have to be revised. (Note that, besides the coherence theory of truth, there are also other theories of truth that are themselves not coherent with respect to the coherence theory of truth.)

Trinajstić thinks that »a single human cannot attain absolute knowledge«. This is certainly true, but I claim that the knowledge of the human race as a whole is not absolute either, since there might be – and certainly are – facts which will never be known to anyone. Absolute electrode potentials of metals are likely candidates of this type of facts, although some theoretical model could be devised to estimate the absolute normal potential of (*e.g.*) gold. Still, the experimental testing of this (estimated) value would most probably be impossible. The epistemological status of unknown facts remains to be clarified.

Science is intimately linked with knowledge, yet the definition of science seems to be extremely difficult. According to Webster's New World Dictionary,[2] science is »....systematized knowledge derived from observation, study, and experimentation carried out in order to determine the nature and principles of what is being studied.« According to Trinajstić: »Science is an ever increasing body of accumulated and systematized knowledge and is also an activity by which knowledge is generated.« But does a book of phone numbers, which is an increasing body of accumulated and systematized knowledge and the activity by which it is compiled, represent science? On the other hand, few people would doubt that Beilstein's compilation of the data on organic molecules (and the work needed to create this book) is a genuine instance of scientific activity.

A »standard view« of science was formulated by Scheffler:[3]

....[The standard view] affirms the objectivity of science...understands science to be a systematic public enterprise, controlled by logic and empirical fact, whose purpose it is to formulate the truth about the world...Observation...supplies the particular empirical facts...People with different theoretical beliefs may observe the same things; shared access to a common word is taken for granted.

Not everybody accepts these views and there is no consensus on which, besides the natural sciences (notably physics, chemistry and biology, and the disciplines dependent on these) plus mathematics and logic, realms of knowledge (including philosophy) should be considered as science. There are several reasons for this; methodological pluralism makes it difficult to arrive at a clearcut definition and by applying the standard view the term science could be used for other non-scientific activities (like criminology or the theory of chess).

In order to solve this problem, the notion that science is a »family-resemblance concept« was proposed.[4] The family-resemblance concept denotes a collection of objects, not because the objects have a single common feature, but because the objects have various partly overlapping resemblances. By accepting this point of view, the characteristics of relevant fields of science could be collected and used to define science, though the problem how to select appropriate »resemblances« would remain.

Similarly, the dichotomy of experiment and theory also poses problems. The first question is which of these is more fundamental, and there are two opposing views – »rationalism« and »empiricism«. A person who subscribes to rationalism will claim that for *ratiocination* it is more important to acquire knowledge than experience, whereas those who subscribe to empiricism will assert that *experience* is more fundamental than theories. In my own view, experience – at least in natural sciences – is more fundamental than theory, since most often theories are created to explain results of already known, empirical facts. Although there are also numerous instances where an existing theory is used to predict previously unexplained or unknown facts, – this is an example of the deductive method – but the theory used to make predictions is itself based on experiments. There are no *a priori* synthetic propositions in natural sciences.[5] The set of *all* theories, practices, skills and intellectual dispositions related to a given field of science is referred to as a paradigm.[6] With the emergence of facts which cannot be explained using the actual paradigm, replacement of the paradigm by a new one becomes inevitable, a process that is often referred to as a scientific revolution.

Concerning research, Trinajstić thinks that »experimental and theoretical research are equally important parts of pure research«.[1] I do agree with this statement, but also claim that this classification is artificial and due to pragmatic reasons – because there are persons who are more interested in experiments than abstract theories and there are also persons whose main interest is in theories. Empirical investigations – at least reasonable ones – are always »theory-laden«, whereas theories depend on experimental facts. It is reasonable to consider chemical analysis as an empirical activity, whereas the derivation of a mathematical formula could be regarded as an example of theoretical activity. Several disciplines cannot be classified into these broad categories. As an example, let us consider researcher X who is interested in obtaining the conformation of a molecule M (to my personal taste, one of the most boring exercises) by performing certain sophisticated *ab initio* quantum chemical calculations. Let us suppose that X obtained the computer program that is needed to accomplish his task from somewhere and starts his calculations by submitting the coordinates of the atoms of M to the computer. After some time, needed for the computations, X obtains a result which may (or may not) agree with reality. Now, does X perform an experiment? Perhaps not, because an experiment would involve actual, physically existing molecule(s) M, and the determination of several properties of M by using a kind of spectroscope or some other experimental device. It may happen (and with quantum chemical investigations it sometimes does happen) that no such molecule M exists. But is X doing theoretical research? After all, X might not be aware of what kind of model his computer program is based on and be still able to perform the calculations. I think the answer is again no, and therefore the concept of theoretical research is vague. Similar reasoning applies to various kinds of »computer experiments«, which are in most cases numerical simulations.

Positivists and many other people (including Trinajstić) consider science as a set of theorems that can either be proved or experimentally confirmed. But neither criterion does guarantee that the result is in accordance with reality.

Positivists also maintain that only those propositions are meaningful that can be proved or experimentally confirmed. This criterion has, however, a serious drawback as we can see by considering a simple example. Let us suppose that X states the following simple hypothesis consisting of a single general proposition involving universals: »all ravens are black«. In order to test this hypothesis, we have to proceed as follows: we observe that $raven_1$ is black, $raven_2$ is black, *etc.* Each »experiment« corroborates the hypothesis. Although the probability that the hypothesis is true will increase with the number of observations, we can never be sure whether there are also non-black ravens. In order to resolve this problem, Popper proposed the »falsification« criterion.[7] According to Popper, the proposal »all ravens are black« can be transformed into a logically equivalent »there is not« type formula which also involves universals: »there are not non-black ravens«. The detection of a single non-black raven – a genuine counterexample – would be sufficient to disprove the theory. A good theory has many possible falsifiers that, however, never materialize. Popper himself considered falsification as a criterion of demarcation [Abgrenzungskriterium] of the (natural) sciences from metaphysics, on the one hand, and from mathematics and logic on the other. Propositions like »there are white ravens« cannot be falsified and are therefore »metaphysical« in Popper's epistemology. Not everybody accepts Popper's falsification criterion as a valid means of demarcation.

Experiments and empirical conclusions have not the same modal status as mathematical theorems. We say that the proposition »2 + 2 = 4« is *necessarily* true, no world could exist in which proposition »2 + 2 = 3« would be true. On the other hand, the proposition »$pV = RT$«, where p denotes the pressure of a gas, V denotes the volume of the container, T is the temperature expressed in K and R is the universal gas constant, has a different modal status, it is *nomically* true, but not necessarily. The reason is that ultimately all theories are based on empirical facts. But empirical facts, as we have seen in the raven example, can never be proved, they can only be confirmed (or disproved) by repeatedly observing the same facts and by using induction to derive conclusions. But, experience does not provide us with the same kind of evidence as do logic or mathematics.

Consider an example constructed by Russel.[5] Assume that there is a chicken – which can think – and it has the following experience: each morning a man arrives and gives him some sort of seed. By induction, the chicken concludes that this will happen each following day, until its master appears with a knife instead of bringing food. As Russel notes, the chicken should have had more precise ideas about the validity of conclusions based on induction.

Trinajstić also considered the process of theoretical research and stated that this includes the following necessary steps: 1. Problem identification, 2. Development of theoretical framework, 3. Numerical approach, 4. Design of computer program, 5. Relevant computation and 6. Interpretation and prediction. All stages entail appropriate documentation which, however, seems not to constitute a separate stage since it accompanies all stages in Trinajstić's delineation. From Trinajstić's discussion it does not follow whether he allowed any of the boxes (stages) to be empty.

First of all, it has to be noted that Trinajstić, by proposing these stages, implicitly advocates the idea that scientific research – and theoretical investigations in particular – *always* follow an identical pattern, which eventually leads to the solution of the problem. Trinajstić's model does not include induction, although it is very often used by researchers, but his model contains all elements needed to do deductive research.[8] The belief that all (essential) discoveries are obtained by the deductive method was also shared by Grünbaum[9]. In connection with the discovery of Einstein's special theory of relativity (STR), Ruzsits[10] remarks:

Grünbaum assumed that Einstein used a set of known principles and assumptions he could prove to be true, together with data from experiments proving the validity of certain assumptions as part of his theory construction ....

Grünbaum's model was dismissed by Hanson, because it is, as Hanson put it, »Logic of a finished research report«.[11] Einstein himself said that he did not use this approach when he discovered the STR, and the Michelson-Morley experiment had only a negligible impact on the development of his ideas.[10] On the other hand, Einstein undoubtedly relied on earlier theoretical work, namely on that by Maxwell, when he deduced some of his results.

Theoretical research and especially stage 2. (Development of theoretical framework) makes extensive use of models. This matter was discussed in detail in a paper by Nikolić and Trinajstić.[12] Trinajstić adopts the following definition: »A model is a representation of something else.« Models are indispensable tools, but to decide whether there are such items postulated in the actual model is often a problem on its own. Example: No one has seen an electron; according to our knowledge, the electron behaves under certain circumstances as a tiny, submicroscopic particle, whereas under other circumstances it behaves like a wave. The assumption (based on classical mechanics) that an electron should either be a particle *or* a wave is clearly wrong. If two (or more) mutually exclusive models are proposed to explain the same phenomenon, other things being equal, the one using the fewest parameters, assumptions, should be preferred. The application of this principle (often referred to as Ockham's razor) in chemistry has recently been reviewed.[13] In any case, models are closely related to analogies. The question of how analogies are related to scientific discoveries was discussed in detail by Rouvray.[14]

There are several beliefs that are widely accepted but which are not true. One is that only those things exist which are studied by science. In order to settle this question, a valid definition of science, which does not exist, would be essential. On the other hand, even if we had such a definition, the view would still be unfounded since it does not (and most probably cannot) follow from experience. The second one holds – and to this Trinajstić also subscribes – that »the value of a theoretical framework depends on its usefulness«[1]. This is a pragmatic view, and one should take into account that »value« is also a vague concept. »Value« in Trinajstić's interpretation could have meant »the number of times the respective result is used or referred to by other scientists or other specialists within a reasonable time interval after it was discovered«. Whether such a »value« is a value indeed, is doubtful. In this connection, it should be mentioned that according to a rather extreme view – instrumentalism – the only value of theories is to make predictions, irrespective of the fact whether the entities or processes whose existence was assumed by a theory do or do not exist. Most scientists, however, are ontologically committed to the existence of those entities or processes they are investigating.

In my opinion, there is no preestablished scheme that would lead to a discovery, although several steps suggested by Trinajstić are essential parts of the process. Therefore, we can conclude this discussion by saying that we do not have adequate ideas how successful research resulting in a discovery should be conducted, but certainly this is not the only basic problem in science, which remains unresolved, including its own definition.

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SAŽETAK

O naravi teorijskog istraživanja: komentari uz Trinajstićev članak

István Lukovits

O nedavno objavljenom članku u ovom časopisu (*Croat. Chem. Acta* **69** (1996) 1013–1022) Trinajstić raspravlja o odnosu teorijskog i eksperimentalnog istraživanja. Ovdje se potpunije raspravlja o nekoliko problema kojih se dotaknuo Trinajstić, a to su: što je znanje, kako definirati znanost te proces teorijskog istraživanja.