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DEPARTMENT OF PHILOSOPHY



STUDIA PHILOSOPHICA

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Special Issue

PROCEEDINGS OF THE THIRTIETH SYMPOSIUM
OF THE INTERNATIONAL SOCIETY
FOR THE PHILOSOPHY OF CHEMISTRY
(1988, 14-20 August 1989)

Edited by David G. Hays, Joseph K. Peterson, and
Richard L. Stroup

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DEPARTMENT OF PHILOSOPHY

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Special Issue:

**PROCEEDINGS OF THE 7th SUMMER SYMPOSIUM
OF THE INTERNATIONAL SOCIETY
FOR THE PHILOSOPHY OF CHEMISTRY
(Tartu, 16–20 August, 2003)**

**Edited by Rein Vihalemm, Joseph E. Earley, Sr.,
Tiiu Hallap**



TARTU UNIVERSITY
PRESS

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Foreword

Some Remarks on the Emergence of Philosophy of Chemistry in the East and West

Rein Vihailemm

This special issue of *Studia Philosophica* is a result of the Seventh Summer Symposium of the International Society for the Philosophy of Chemistry (ISPC) held at the University of Tartu on August 16–20, 2003. The philosophy of chemistry is a new, rapidly progressing branch in philosophy of science. In addition to being interesting in its own right, it plays an essential role in contemporary philosophy of science generally. In order to characterize the current state of affairs in this new branch of inquiry, let me say some words about major conferences and publications in this field, and also about its emergence both in international and local — that is, Estonian — context.

The ISPC was founded in 1997 (in Ilkley, UK). Since 1999, its official journal is *Foundations of Chemistry* published by Kluwer; the editor-in-chief of this journal is Eric R. Scerri from the University of California at Los Angeles. Another international journal *Hyle* which is also devoted to philosophy of chemistry is being published electronically since 1995 already, the editor-in-chief being Joachim Schummer from the University of Karlsruhe. Since 1997, a printed version of this journal exists as well.

The ISPC has annually arranged summer symposia (1997 — Ilkley, UK; 1998 — Cambridge, UK; 1999 — Columbia, USA; 2000 — Poznań, Poland; 2001 — Loughborough, UK; 2002 — Washington, USA; 2003 — Tartu, Estonia; 2004 — Durham, UK). Papers presented to the Columbia, Poznań, and Washington symposia

are published as (Baird et al. *forthcoming*, Sobczyńska et al. 2004, Earley 2003). Even before the ISPC was founded, international conferences on philosophy of chemistry were held in the early 1990s, and several proceedings of these events were published as well (for the overviews and references see van Brakel 1999: 112–113, 2000: 37–40, Scerri 2003: 3–6). The meeting which took place in March 1994 at the London School of Economics was called the First International Conference on the Philosophy of Chemistry. In July 1994 the first International Summer School of Philosophy of Chemistry was organized at the Bradford College in Ilkley. In that year several other international meetings on philosophy of chemistry were also held, and it seems right to say that philosophy of chemistry was born in 1994 (van Brakel 1999: 112, 2000: 38, Scerri 1999: 107). Since 1990 more than 500 papers and about 40 monographs and collections have been published on philosophy of chemistry (Schummer *forthcoming*).¹

However, if we do not limit ourselves to the English-speaking world of philosophy, we shall have to say that in fact philosophy of chemistry began to emerge as early as in the 1960s in the Soviet Union and Eastern Europe (see also van Brakel 1999: 122–129, 2000: 22–34). Two all-union philosophical conferences devoted to issues concerning chemistry took place in the 1970s and 1980s (Rostov-on-Don, 1972; Moscow, 1980).² In 1981, a bibliography of main Soviet literature (from 1945 to 1980) on philosophical problems of chemistry was published (see *Filosofskiye* 1981). The bibliography lists 565 publications (all in Russian), including 60 monographs or collections from the period 1960–1980. Earlier publications should be ignored because during this earlier period the Stalinist ideological pressure

¹ A regularly updated online bibliography maintained by J. Schummer is available at: <http://www.hyle.org/service/biblio.htm>.

² In the program of the Rostov conference there were altogether 23 presentations (*Filosofskiye* 1972), including papers by two authors who have also contributed to the present volume — A. Pechenkin and R. Vihalemm (see *Filosofskiye* 1972: 3–4, 14–15). The program of the Moscow conference lists 31 titles of papers; again, A. Pechenkin and R. Vihalemm were among the participants of the event (see *Programma* 1982: 1, 2).

was fatal for real philosophy. (For a general characterization of Soviet philosophy of science see Graham 1987; chapter 9 is devoted specifically to chemistry. Graham's outlook has been corrected in some points by A. A. Pechenkin (1995)). One of the distinguished authors in the field of philosophy of chemistry from the second half of 1960s–1980s was Alexander Pechenkin whom we mentioned already: he has written three monographs on philosophy of chemistry (Pechenkin 1976, 1986, Kuznetsov & Pechenkin 1978).

Since 1965 philosophy of chemistry also began to emerge in Estonia which was part of the Soviet Union until 1991. The first paper on philosophy of chemistry devoted to the interrelations between chemistry and quantum mechanics was published in 1965 by R. Vihalemm in the series *Acta et Commentationes Universitatis Tartuensis* (Vihalemm 1965). Afterwards, 7 more papers on philosophy of chemistry were published by the same author in the same series; in addition, he published 20 works (before 1991) in other Soviet (but also in Polish and Yugoslav) journals or collections, mainly in Russian, but also a few articles in Estonian and in English (the 8th International Congress of LMPS paper — Vihalemm 1987)³. Vihalemm also published a book (1981) which philosophically analyzed the emergence of chemistry as a science. Some works concerning philosophy and methodology of chemistry were also published by other Estonian authors, both philosophers (L. Näpinen) and chemists (V. Palm). A general overview of philosophy of science in Estonia from Soviet times until nowadays is available in Rein Vihalemm's book (2001); the book also contains some articles (by E. Lõhkivi, L. Näpinen, V. Palm, V. Past, R. Vihalemm) concerning philosophy and history of chemistry. Since 1994 Estonian philosophers and chemists have also contributed to the development of philosophy of chemistry on the international level. This brings us already to the ISPC Tartu conference.

³ By the way, reference to this Congress is absent in (van Brakel 2000: 38, *Block 1–12*). At that Congress several papers on philosophy of chemistry were presented — e.g., by F. Felecan (Romania), and I. Stengers (Belgium) & L. Chertok (France). See Programme 1987: 58, 59, 93.

At this conference 6 Estonian philosophers and chemists welcomed 16 guests from 9 countries. During four days 19 presentations were discussed.

At the opening session (*Session Chair — R. Vihalemm*), after an address of welcome by the Dean of the Faculty of Physics and Chemistry, Professor Jaak Järv, a lecture “Wilhelm Ostwald and Physical Chemistry at the University of Tartu” was given by Vello Past (Emeritus Professor of Physical Chemistry). In a way, this presentation marked the 150th birth anniversary of Wilhelm Ostwald — until now the only alumnus of Tartu University who has been awarded the Nobel Prize. Professor Past kindly agreed to write an article for this volume on the role of Wilhelm Ostwald and of the University of Tartu in the emergence of physical chemistry.⁴

Further speakers and the titles of their presentations in the actual order were as follows:

Session 1, Chair — E. Lõhkivi:

Paul Bogaard (Mount Allison University, Canada) — “G. N. Lewis and the Reconciliation of Theoretical Chemistry”;

Michael Akeroyd (Bradford College, UK) — “Predictions, Retrodictions and Chemistry: A 20th Century Example”.

Session 2, Chair — M. Akeroyd:

Claus Jacob (University of Exeter, UK) — “Historical and Logical Aspects of Chemical Arguments”;

Viktor Palm (University of Tartu, Estonia) — “Computerized System for the Automatization of the Sound Procedures of the Methodology of Science”.

⁴ Vello Past has written on this topic in some earlier publications already (see especially: Past 2001). Wilhelm Ostwald’s contribution to the philosophy of chemistry is analyzed, e.g., in (Vihalemm 2004).

Session 3, Chair — J. E. Earley, Sr:

Slawomir Michalak (University of Medical Sciences, Poznań, Poland) — “Concentric Patterns in the Brain: A Thermodynamic Aspect of Disease”;

Alexander A. Pechenkin (Institute of the History of Science and Technology, Moscow, Russia) — “How to Understand the History of the Belousov-Zhabotinsky Reaction”;

Leo Näpinen (Tallinn University of Technology, Estonia) — “The Understanding of the Relationship Between Man and Nature in Physics and Chemistry”.

Session 4, Chair — R. F. Hendry:

Joseph Simonian (University of California, Santa Barbara, USA) — “Water Ain’t Necessarily H₂O”;

Jaap van Brakel (Catholic University of Leuven, Belgium) — “On the Inventors of XYZ”.

Session 5, Chair — P. Needham:

Robin F. Hendry (University of Durham, UK) — “Reference and Chemical Kinds”;

Rom Harré (Georgetown University, Washington D.C., USA and University of Oxford, UK) — “Essences Revisited”.

Session 6, Chair — J. van Brakel:

Joseph E. Earley, Sr. (Georgetown University, Washington D.C., USA) — “Why There Is No Salt in the Sea”;

Paul Needham (University of Stockholm, Sweden) — “Mixtures and Modality”.

Session 7, Chair — R. Harré:

Ko Hojo (Chiba, Japan) — “Kitaro Nishida Considered in Philosophy of Chemistry”;

Werner Brandt (University of Wisconsin, Milwaukee, USA) — “Chemistry in Liberal Education: the Curse of Oversimplification”.

Session 8, Chair — A. A. Pechenkin:

Endla Lõhkivi (University of Tartu, Estonia) — “What Models Can Do: An Empirical Study of the Use of the Concept of Model in Research on Biosensors”;

Peeter Määrsepp (Audentes University, Estonia) — “Chemistry as an Independent Science”;

Rein Vihalemm (University of Tartu, Estonia) — “Philosophy of Chemistry and the Image of Science”.

Four of the papers delivered at the Tartu conference were dedicated to the work of another Nobel Prize winner — the Belgian physical chemist and philosopher Ilya Prigogine. As Prigogine (1917–2003) had died in Brussels on May 28, 2003, *Session 3* of the conference (chaired by Professor Earley), where three of the aforementioned four papers were presented, was called “The Ilya Prigogine Memorial Symposium”. Papers by A. A. Pechenkin, S. Michałak, and L. Näpi-nen from *Session 3*, together with P. Määrsepp’s paper from the last session, are collected in the present volume under the title of that memorial symposium. Professor Earley who knew well Professor Prigogine as a collaborator and friend, was happy to be the editor of that part of this volume. He also contributed a short piece on Prigogine’s life and work as an introduction to it.

Among the presentations in sessions 4–6 there were six papers which analyzed a common topic — the problem of natural kinds in chemistry. These papers are not part of the present volume, since it was considered reasonable to submit these papers for publication in a special issue of the *Foundations of Chemistry* (Vol. 7, Issue 1, 2005, pp. 1–118). Rein Vihalemm’s Tartu paper will be hopefully published in another special issue of the same journal.

As to the remaining papers of the Tartu symposium, five more articles were submitted for publication in *Studia Philosophica*. The papers by Michael Akeroyd, Claus Jacob, and Endla Lõhkivi analyze some chemical examples or case stories from historical, logical or methodological viewpoints. Werner Brandt’s paper considers the interrelation between liberal education and philosophy of chemistry. The article by Ko Hojo introduces to Western philosophers of science

(and chemistry) some concepts present in the philosophy of a distinguished Japanese philosopher Kitaro Nishida (1870–1945).

Acknowledgments

Finally, as chairman of the editorial board of this issue of *Studia Philosophica* and as chairman of the local organizing committee of the ISPC Tartu Symposium, I would like to thank all who helped to arrange this event and contributed to the production of the present volume. The symposium was organized by the Chair of Philosophy of Science of the Department of Philosophy (chairman of the organizing committee — Rein Vihalemm) in cooperation with the Department of Chemistry of the University of Tartu; it was supported and sponsored by the Office of the Rector, by the Department of the Humanities and Social Sciences of the Tallinn University of Technology (member of the organizing committee — Ülo Kaevats), by the Audentes University (member of the organizing committee — Peeter Mürsepp), and by the City Government of Tartu. Last but not least, special thanks to the secretary of the local organizing committee, Associate Professor Endla Lõhkivi, to the special editor of this volume, Lecturer Tiiu Hallap, and to the editor of Part 2, Professor Joseph E. Earley, Sr. My work in the production of this volume was partially supported by the ESF grant no. 5804.

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PART I

Historical, Logical, and Methodological Aspects

Wilhelm Ostwald and Physical Chemistry at the University of Tartu

Vello Past

Wilhelm Friedrich Ostwald (1853–1932) was one of the most prolific, imaginative and influential scientists of his time. He was appreciated as the leader in the establishment of physical chemistry as a separate discipline. In 1909, Ostwald was awarded the Nobel Prize in chemistry for his achievements in the study of catalysis, chemical equilibrium and reaction kinetics.

In Ostwald's life, three towns — Riga, Tartu and Leipzig — played an especially important role. In Riga he was born 150 years ago (on September 2, 1853), in the family of a German entrepreneur. He graduated from Riga's *Realgymnasium* which gave him a very good preparation for his later studies at the university. Young Ostwald ardently wished to become a researcher-chemist. He believed that the chemistry department at the University of Tartu (at that time Dorpat) was a suitable place for realizing this dream.

The last quarter of the nineteenth century witnessed a fruitful stage in the development of physico-chemical research. The emergence of physical chemistry as a separate discipline culminated in Germany, in 1887–1888. However, the formation of this new branch of science was facilitated by physico-chemical research at universities in various countries. In this respect the University of Tartu also made a remarkable contribution (Past 2001: 38).

The year 1850 marked a turning point in the development of chemistry in Tartu when an independent Chair of Chemistry as a department of the new Faculty of Physics and Mathematics was

established. The University began to train chemists and to award chemist's diplomas to the graduates of the new department. From the very beginning, favorable conditions for research in chemistry, and especially in its new fields, were created at the department. It was Carl Schmidt (1822–1894), professor of chemistry in Tartu for 40 years, whose merits were the greatest. Schmidt was not only a first-rate scientist, one of the best analysts of his time, but also a highly esteemed teacher who trained numerous outstanding chemists in Tartu.

Wilhelm Ostwald was a student of the chemistry department of Tartu University from 1872 to 1875. The head of the department, Carl Schmidt, became for Ostwald a model of an ideal professor and remained such until the end of his life. When Ostwald himself became a professor he tried to imitate his teacher. Ostwald liked Schmidt's lectures on the history of chemistry above all, and he visited those lectures regularly although in other cases he preferred to read textbooks instead of attending lectures.

Another person whose influence on Ostwald was also very strong was the instructor of practical work in chemistry, assistant Johann Lemberg (1842–1902). Lemberg was an unusual person. Students were impressed by the erudition of the young instructor, his truthfulness and devotion to laboratory work. Lemberg carried out a profound research of chemical transformations of natural silicates and was the first to use the law of mass action for the explanation of his results. As a teacher he made students use several physical methods of measurement, thereby stressing the importance of quantitative relations in chemistry. Later Ostwald declared that a world of measurements had opened up in the university laboratory which gripped him immensely (Ostwald 1926: 98–99). Under Lemberg's influence inquisitive students began to understand the essential role of chemical equilibrium in science.

Already as an undergraduate Ostwald was keen on scientific research. At Lemberg's suggestion he took up research into the equilibrium of the hydrolysis reaction of bismuth chloride. This became the topic of his candidate's thesis. The publication of a review of his thesis in an international journal (Ostwald: 1875) gave the author new energy and confirmed his decision to persist in the chosen physico-

chemical field. This article was the first published work among Ostwald's numerous writings and as such was cherished by the author.

Upon his graduation from the university Ostwald was 21 years old, but in spite of his youth he had a clear vision of the direction of his further research on the boundary between physics and chemistry. He gladly accepted an invitation to work as a research assistant at the department of physics in the University of Tartu. This post enabled him to update his knowledge of mathematics and physics which he considered very important for his future scientific career. Head of the department, professor Arthur von Oettingen (1836–1920), was convinced that physics and chemistry should mutually approach each other. He supported Ostwald's steps in this direction. Participation in the workshops and discussions with physicists provided Ostwald with a physical conception of the world and inspired him to improve his knowledge of that field (Ostwald 1926: 111).

In the department of physics Ostwald began extensive research on chemical affinity with the aim of quantitative determination of affinity coefficients of acids in their reactions in solutions with a base or with a salt of another acid. Once again we can note the influence of Johann Lemberg who studied chemical affinity in geochemical transformations of silicates and alumosilicates under the influence of salt solutions. In particular, Lemberg initiated a physico-chemical approach to the investigation of chemical processes that completely superseded Carl Schmidt's scientific direction of chemical analysis in the department of chemistry in the 1880s (Past 2001: 40). It is remarkable that Ostwald had enough boldness and self-confidence to take up the rather complicated problem of affinity. Chemical affinity linked together the general regularities of chemical reactions — chemical equilibrium, reactivity and reaction kinetics.

Ostwald pioneered the important measurement technique of using changes in physical properties (such as volume and refractive index) to investigate chemical reactions in a quantitative way. Being a skilful experimenter, he was able to construct the measuring equipment himself. His work on chemical affinity gave good results. On the basis of this research he wrote and successfully defended his master's thesis in 1877 and, a year later, his doctoral thesis (Ostwald 1878).

During the Tartu period (1875–1881) Ostwald published a total of 12 articles (Walden 1904: 109–110). The main result of these papers was the determination of the affinity coefficients of about 20 acids. The author presented a series of acids which was in general very close to the acidity scale proposed later on the ground of the theory of electrolytic dissociation. The sequence of acids that Ostwald determined by measuring volume effects essentially coincided with the results of thermo-chemical measurements made by the Danish chemist Julius Thomsen. However, no answer was provided to the question why compounds displayed acidic properties or why the intensity of these properties was so different for different compounds. The answer was given by the Swedish chemist Svante Arrhenius in the following decade.

The favorable atmosphere in the University of Tartu turned Ostwald into an independent scientist in the field of physical chemistry. His growth to maturity culminated with the defending of his doctoral degree on the 9th of December, 1878. Later on in his life, Ostwald always celebrated that day of reaching the highest scientific pinnacle. His former student, a Latvian Paul Walden, devoted a monograph on Ostwald to the occasion of the 25th anniversary of this event (Walden 1904).

The master's degree gave Ostwald the right to lecture at the university. This was the beginning of his teaching career. To qualify as a privatdozent, Ostwald had to prepare a two-hour probationary lecture with the title "Physical chemistry. The theory of affinity". The amount of literature necessary for preparing the lecture was fairly extensive, but Ostwald displayed remarkable skills in systematizing various materials and presenting them from a certain point of view. After the successful delivery of the probationary lecture in the beginning of 1878 Carl Schmidt suggested to Ostwald that he should write a textbook of general chemistry. Ostwald was inspired by this suggestion and immediately started to work out the plan of the book and to collect material. The fundamental two-volume manual, which was begun in Tartu and completed in Riga, was published in Leipzig under the title "Lehrbuch der allgemeinen Chemie" (Ostwald 1885, 1887).

The defense of the doctoral thesis did not change Ostwald's academic position at the University of Tartu. In 1880 he became a laboratory assistant of the chemistry department. His qualification would have enabled him to become a professor of chemistry, but the post was occupied by Carl Schmidt. In the autumn of 1881 Schmidt received a letter from the Riga *Polytechnic*, requesting him to recommend one of his students for a vacant professorship in chemistry in Riga. Schmidt recommended Ostwald as an entirely suitable scientist for the vacancy. He predicted a brilliant scientific career for his most gifted student. As we know now, the prediction came true to the full extent. As a professor of chemistry at the Riga *Polytechnic* from 1882 to 1887 Ostwald won wide recognition in the scientific world. Since 1887 Ostwald worked as a professor of physical chemistry at the University of Leipzig. Here he became the acknowledged leader of a school of scientists with the world's largest membership. In the University of Leipzig Ostwald, with his co-workers, made his main contributions to the development of physical chemistry. He retired at the age of 53 and spent his remaining years working as a "free" professor at his estate in Grossbothen (near Leipzig). He died in 1932.

The scientific trend initiated by Johann Lemberg and Wilhelm Ostwald in Tartu was fruitfully developed by Gustav Tammann (1861–1938) in the last two decades of the 19th century. Tammann studied physics (1879–1880) and chemistry (1880–1882) at the University of Tartu. Here he defended his doctoral thesis on the study of the metamery of metaphosphates (1890). In the years 1892–1902 Tammann was professor of chemistry at the University of Tartu. In his early works, which were mostly devoted to the experimental study of the principal aspects of the theory of solutions, he established some important relationships between the concentration of a dissolved compound and the observed physical effects. From the mid-1890s Tammann, together with his co-workers, undertook a thorough investigation of the problems of heterogeneous equilibrium. Investigating the properties of ice at high pressures, he detected two new modifications of ice (ice II and III).

During his Tartu period (1885–1902), Tammann wrote 68 scientific articles and the monograph “Kristallisieren und Schmelzen”, printed in Leipzig (Palm 1976: 180). His research during this period covered a wide range of problems not only in the domains of physical and inorganic chemistry, but also, for example, in physiological chemistry. In this latter field Tammann analyzed physiological problems from the standpoint of physical chemistry, e.g. emphasizing the role of osmosis in the functioning of an organism. His studies of enzymatic reactions are even more widely known as the first attempt to view biocatalytic processes from the standpoint of physical chemistry.

At the end of 1902 Tammann accepted the offer made by Walter Nernst and became the director of the newly established Institute of Inorganic Chemistry at the University of Göttingen. He died as a world-known scientist in Göttingen at the age of 77.

After Tammann’s departure from Tartu a group of his former students (Aleksandr Bogojavlenski, Georg Landesen, Nikolai Kuldašev, Reinhard Hollmann, Vassili Borodovski, Johannes Narbutt) continued research on those topics which had interested Tammann. Their activities marked the end of a significant stage in the development of physical chemistry at the University of Tartu. The university had won wide recognition not only as a research center but also as an educational institution. Success of the graduates of the chemistry department in the field of physical chemistry can be accounted for by the peculiarity of the curriculum here, with the main subjects alongside chemistry being mathematics and physics. According to Tammann (1901: 5) education given at the University of Tartu was chemico-physical, not naturalistic as in the universities of Russia, and also not purely chemical as at foreign (German) universities.

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Predictions, Retrodictions and Chemistry: A 20th Century Example

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Introduction

The main battleground for the debate between the retrodictivists and the predictivists in chemistry has been concerned with Mendeleev's famous predictions and their effect or otherwise on the acceptance of the Periodic Table. However, it is rare for predictions to be published in such a detailed form prior to corroboration. The author looks at a 20th century example where an individual scientist transferred allegiance to a speculative new theory, following some predictive success, although the majority of his colleagues preferred to support the orthodox theory, since this still retained overall evidential support.

While retrodictivists can allow that it is rational for ambitious innovatory scientists to propose and pursue theories which possess less empirical support than the currently accepted theory, just in case future evidence will generate overall accommodatory support, they have not addressed the problem of whether it is rational for other scientists to transfer their support *after* the novel theory has had *some* empirical success, but *before* it explains *more* than the conventional theory. The point is that these recent converts have little to gain and much to lose with their academic status.

The author gives some theoretical reasons why recently collected empirical data generated from testing specific predictions should be given more weight than the 'old data' supporting the conventional

transferring allegiance five years after a controversial new theory had first been proposed.

Paul Bartlett, a US physical organic chemist, publicly supported the then controversial Hughes-Ingold S_N1 mechanism in a paper published in 1939. However, the published predictions made by Hughes-Ingold were less specific than those made earlier by Mendeleev concerning *eka*-aluminium, *eka*-boron, *eka*-silicon, and the author devotes time to discussing the significance or non-significance of this particular aspect.

The predictivist account¹

Usually, when a new theory is proposed, the originator feels that the new theory (NT) solves a problem that is an anomaly for the current theory (CT) — a problem that he/she considers important. The originator thinks that this is an indicator of the possibility that that NT might supplant CT in the future, and submits a paper for publication. If the referees agree, the theory is published in a prestigious journal. However, it is unlikely that NT accommodates all the existing data accommodated by the older CT, since then it would have been devised earlier and it would now *be* the current theory. Had gallium, scandium and germanium been isolated in the early 1860s, then Newlands would have invented the Mendeleev periodic table.

Anyway, Nobel Laureate Francis Crick once famously remarked that he did not trust a theory that ‘explained all the data’, because ‘some of the currently accepted data is wrong’. It is a commonplace in science that old experiments are often reworked, when it is noticed that their empirical conclusions conflict with new theories that are otherwise highly successful. The experiment which is repeated using modern, more sophisticated apparatus, usually indicates that the early data was inaccurate and that the observed new corrected data supports the new theory. Data accumulated *recently* is more likely to be accurate than older data, since experimental techniques will now be more accurate. In addition, the data accumulated through testing

hypotheses and predictions is also likely to be even more accurate than data *not* accumulated through such testing, since *greater care* will be taken with the experimental conditions in excluding external 'noise' and 'complicating effects'. Predictive methodology is a relatively simple, painless way of selecting the more reliable data from the less reliable data, when analysis of the total sum of the data does not yield clear-cut decision between two or more competing theories. *Recent data acquired via the route of Popperean 'severe testing' is likely to be more accurate than data acquired in the past. It should be therefore given greater weight as compared with data acquired via any other route.*

Suppose NT achieves some qualified acceptance for its accommodation of the anomalies besetting CT and its accommodation of a large body of facts also accommodated by CT. However, its overall accommodatory power will still be less than that of CT because of its novelty. Why should anyone originate or publish a theory that accommodates fewer facts than the currently accepted theory? It has been observed that this could be a rational exercise for some young scientist ambitious for a Nobel Prize, establishing their priority if the theory later supplants CT, but most of this scientist's colleagues will play a more cautious game, continuing to develop CT. However, after some of NT's predictions have been corroborated (some of NT's retrodictions, which have 'accidentally' become temporal predictions, must conflict with CT, otherwise NT would not be a different theory) some other scientists switch allegiance from CT to NT although the accommodatory power of NT is still lower than that of CT. Why do they do this? They will not win future Nobel Prizes for this as they did not invent the theory. Why do they risk the opprobrium of their colleagues and (in the short run at least) diminish their career prospects? *Because they feel that the successful predictions are a valid indicator of future promise, that NT has passed severer tests than has CT for all its accommodations, that they are making a shrewd decision in abandoning the sinking ship of the old CT.*

The Hughes and Ingold theory of aliphatic organic mechanism

Prior to 1920 there had been no satisfactory theory of the actual mechanism of the millions of organic reactions that had been catalogued. After 1920, with the development of Quantum Mechanics, a 'transition state' theory was developed which suggested that the minimum energy state for an 'activated complex' (i.e. the entity with the 'attacking' group and the 'leaving' group both partially bonded to the same carbon atom) required 'attack from the back' by the incoming group, i.e. the incoming group, carbon atom and outgoing group all lay temporarily on a 180° line. Empirical evidence that this occurred in a large number of 'saturated' aliphatic organic reactions was presented by Paul Walden and his co-workers.

However, some molecules possessed structures where this convenient 'attack from the back' was precluded. Most organic chemists assumed that some 'front side' attack must be occasionally allowed, but the UK chemists Hughes and Ingold (1933, 1935) proposed a novel 'duality of mechanism' approach: when the presence of methyl groups on the active carbon atom physically hindered the approach of an attacking atom or group, these methyl groups would tend to donate electrons towards the active carbon atom and favour the dissociation of the molecule into a positive fragment and a negative fragment. The positive fragment would then react with the 'incoming group' in a heterolytic, as opposed to a homolytic, mechanism. Although a few organic aliphatic reactions were known to proceed through an ionic mechanism (e.g. camphyl chloride with aqueous silver nitrate), the majority of chemists had an aversion to the idea of ionic mechanisms under 'normal conditions' in 'normal solvents' such as 80:20 ethanol-water mixtures.

From 1933–1938 the Hughes-Ingold proposals were known as the 'English Heresy' and leading US physical organic chemists such as Hammett, Roberts and Winstein were vociferous in their opposition, proposing new models to support the conventional 'transition state' theory while conceding some of the objections of Hughes-Ingold to its original formulation. However, in 1939, one leading US physical

organic chemist broke ranks and published a paper with new results that supported the Hughes-Ingold theory. Following the ideas expressed in the Introduction, I claim that this was because the results supported the predictions of the Hughes-Ingold theory. For more historical background details see Akeroyd (2000).

Paul Bartlett's research

Paul Bartlett and his research student Laurence Knox were well aware of the Hughes-Ingold model, but they were particularly interested in the mechanism of the so-called 'Walden Inversion'. When a molecule containing an 'asymmetric carbon atom' (i.e. a carbon atom with four different functional groups attached to it) undergoes nucleophilic substitution, the product will show significantly different optical properties with respect to polarised light. $X-CR_1R_2R_3$ yields $R_1R_2R_3C-Y$, whose shape cannot be superimposed over the original.

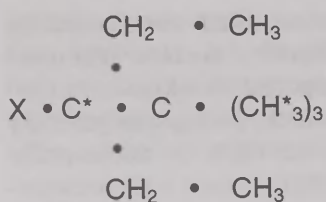
Bartlett was also interested in the theoretical reason underlying 'Bredt's Rule', the rule that functional groups bonded to the 'bridge-head carbon atoms' became very inactive and difficult to substitute. 'Bridge-head carbon atom' occurs in a bicyclic ring structure, i.e. a structure where the majority of a chain of saturated carbon atoms are located in a ring structure, but there exists a secondary cross linking chain. In the introduction to their classic paper Bartlett and Knox (1939) stated: 'The present work is to test the hypothesis of the universality of the Walden Inversion...', but indirectly it was to test the predictions of the Hughes-Ingold theory, since if inversion of configuration (whether detectable or not) was synonymous with transition state theory, then some different mechanism must be postulated to accommodate the recognised existence of non-inverted products.

Some important background work prior to Bartlett's investigations was performed by another US organic chemist, Frank Whitmore and his colleagues. Whitmore once wrote to Ingold (see Ingold 1969: 742-3, note 78) stating that he privately supported ionic

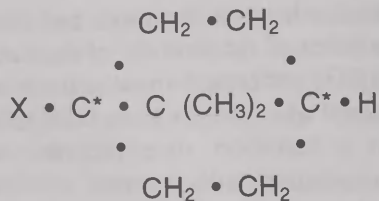
mechanisms at the time, but his public views were constrained by referees of the *Journal of the American Chemical Society*. Whitmore (1933) performed investigations on the compound then known as neo-pentyl chloride, formula $(\text{CH}_3)_3\text{CCH}_2\text{Cl}$, which, perhaps surprisingly to a transition state theorist, was very resistant to nucleophilic substitution under 'normal' conditions and then reacted with considerable rearrangement when subjected to forcing conditions that might conceivably encourage an ionic type mechanism. Because the bond angle in 4-valent carbon is $109^\circ 28'$, the backbone chain of carbon atoms in a so-called 'straight chain' compound is actually zig-zag and space-filled models of this molecule indicate that 'attack from the back' on the carbon atom linked to the chlorine atom is hindered by one of the nine hydrogen atoms linked in the three terminal methyl groups (see diagram on p. 32).

However, when neo-pentyl chloride *did* react, under conditions which, according to the Hughes-Ingold theory, encouraged an ionic mechanism, the main product was *t*-amyl alcohol $(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{CH}_3$, and not neo-pentyl alcohol as expected. What Bartlett and Knox required as a substrate was a compound similar in structure to neo-pentyl chloride but possessing no alpha hydrogen atoms that permitted easy rearrangement. Such a compound had recently been isolated as a by-product of a reaction involving ethyl magnesium bromide and tri-methyl ethyl chloride by Whitmore and co-workers (1939).

Its modern name is 2,2 dimethyl-3-ethyl-3-chloro pentane, but Bartlett referred to it as tertiary butyl di-ethyl chloride. Using 'space filling models' cited by Stuart (1934), rather than the old fashioned 'ball and stick models', Bartlett and Knox showed how effectively the beta hydrogen atoms shielded the target carbon atom from the approach of any potential attacking reagent. Consideration of the *paper* representation of the molecules of tertiary butyl diethyl chloride with the caged molecules of 1-apocamphyl chloride and bornyl chloride does not bring out their similarity of appearance in three-dimensional space.

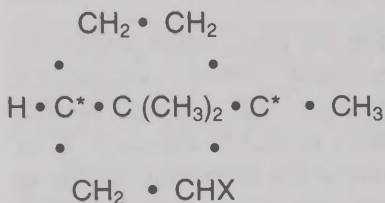


Tertiary butyl diethyl chloride (X = Cl)



1-apocamphyl chloride (X = Cl)

Note that in a space filled model, one of the nine starred hydrogen atoms is physically close to the starred C atom.



Bornyl chloride (X= Cl). Note X is substituted adjacent to a 'bridgehead' (starred) carbon atom.

Although complicated to synthesise from scratch, bornyl chloride was well known to organic chemists as a product that could be isolated from the naturally occurring product camphor. The 'caged and bridgehead' molecule of apocamphyl chloride was not known at the time to be unreactive, since only the 'parent' hydrocarbon apocamphane was known, however, the 'caged' but 'non-bridgehead' bornyl chloride was known to be unreactive to 'normal' reagents but react slowly with silver nitrate solution via an assumed ionic mechanism (Meerwein and van Emster 1920).

Bartlett and Knox decided to perform kinetic studies on the rates of hydrolysis of the three substances: officially (from the point of view of the referees of the paper) to directly test the hypothesis of the

universality of the Walden Inversion, but also (indirectly) to test the predictions of the Hughes-Ingold theory. This theory, according to the general principles expounded by the originators, would predict that tertiary butyl diethyl chloride would hydrolyse much more readily than the caged molecules, and somewhat more readily than the 'parent' tertiary congener: tert-butyl chloride $(\text{CH}_3)_3\text{CCl}$ which had been studied in 1933.

In a comment anticipating Crick's later aphorism relating to the proportion of old data that is wrong, Whitmore (1933) wrote scathingly:

Tissier (1893) and Richard (1910) prepared what appeared to be neo-pentyl chloride. The former claimed that the monochloride obtained by the chlorination of neo-pentane was identical with that obtained from neopentyl alcohol and dry hydrogen chloride, and that it decomposed on distillation. It has recently been found by this writer that neo-pentyl chloride cannot be prepared from the alcohol.

Bartlett's results and discussion

Bartlett was the first organic chemist to synthesise quantitative bulk amounts of tert-butyl diethyl chloride and 1-apocamphyl chloride for kinetic studies. He found that tert-butyl diethyl chloride hydrolysed in an 80:20 ethanol:water mixture at 25°C thirteen times more rapidly than tert-butyl chloride, and 30% more rapidly than tert-amyl alcohol, while 1-apocamphyl chloride and bornyl chloride were unaffected.

However, when 1-apocamphyl chloride and bornyl chloride were both treated with silver nitrate solution at 25°C, 1-apocamphyl chloride was unaffected, but bornyl chloride lost 22% of its chlorine within 5 minutes and 84% within 60 minutes.

These results are difficult to explain on the hypothesis that the Walden inversion is the universal mechanism for substitution at saturated carbon, since we would expect the solvolysis rates of the

three compounds to be approximately comparable. Nor are they explicable by making the assumption that the 'Walden Inversion' with its 'backside attack' is the preferred mechanism, but when steric factors come into play, 'frontside attack' becomes the option of last resort: the chlorine at the 'bridgehead' of 1-apocamphyl chloride should be more exposed to attack, and hence more reactive than the chlorine atom linked to the carbon atom adjacent to the 'bridgehead' in bornyl chloride.

But the Hughes-Ingold theory would, *per contra*, lead us to expect that bornyl chloride is more reactive than 1-apocamphyl chloride, since the extremely rigid structure associated with the 'bridgehead' carbon hinders the formation of the planar positive ion postulated by quantum mechanical considerations, if the positive charge is located on carbon atom C*.

In the final paragraphs of their paper, Bartlett and Knox finally cautiously introduced the reader to the heretical Hughes-Ingold theory, and almost apologetically indicated how this theory would predict an order of reactivity tert-butyl diethyl > tert-butyl >> bornyl >> apocamphyl. They also showed how all this was consistent with the recent results of Levy and Brockway (1937) in a paper on inorganic chemistry published in the *Journal of the American Chemical Society*. The electron deficient species BH_3 , BF_3 and $\text{B}(\text{CH}_3)_3$ were shown by modern physical sensors to adopt a planar configuration with bond angles of 120° : by analogy the hypothetical $\text{CR}_1\text{R}_2\text{R}_3^+$ ion should also be expected to adopt a planar configuration. Bartlett and Knox's conclusions were suitably tentative (as befits the etiquette of an empirically based science), but to other leading workers in the field the indication was clear: Bartlett had transferred allegiance to a younger rival theory because of its recent successful predictions. He had assigned greater weight to *recent* empirical evidence obtained under rigorously controlled conditions rather than to *old* empirical evidence obtained under less rigorously controlled conditions.

Concluding remarks

Retrodictivist philosophers might argue that since Hughes and Ingold had not published any prior predictions concerning caged molecules and their potential reactivity on their theory and, since Bartlett and Knox chose to publish both the predictions and the successful corroborations in the same paper, then this example does not support the traditional predictivist methodological position. In the case of Mendeleev's Periodic Table, it is possible to argue (with Scerri and Worrall 2001) that the sum of total evidence by 1882 supported the concept of a Periodic Table whilst the earlier 1870 version was not so well supported (i.e. gallium and scandium were still unknown), and that the famous Mendeleev predictions were therefore an irrelevant factor in theory choice. It is, however, debatable as to whether the 'sum total of evidence' in 1882 supported the Periodic Table as compared with the 'sum total of evidence' in 1870, if one incorporates the then recently discovered rare earth elements into the system (Akeroyd 2003). However, no one could seriously consider that the 'sum total of evidence' supported the Hughes-Ingold theory as early as 1939, even after the incorporation of Bartlett's work on caged molecules. It is possible for retrodictivists to argue that the attitude of other US based physical organic chemists changed towards the Hughes-Ingold theory after 1940 on the basis of total evidence, since the English chemists published a powerful series of papers in 1940 containing large amounts of novel data that they had researched in the time period 1938–1940. But it is not possible to argue that the work of Bartlett and Knox on caged molecules swung opinion towards the S_N1 theory on any retrodictivist criterion.

Note

1. This section was first published in Akeroyd (2003). Thanks are due to Kluwer Academic Publishers for permission to reproduce it here.

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Some Remarks on Chemical Arguments

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Introduction

Philosophical reflection has little tradition within chemistry and attempts to bring philosophical thoughts into the realm of chemistry frequently have to be justified. In this respect, chemists tend to request 'added value', implying that philosophy is only interesting for chemists if it can be of direct use, i.e. tell chemists something they don't already know from chemical research, experience or common sense. The idea of a 'philosophy free' chemistry is, however, a very unfortunate myth. As we will see, elements of philosophy are omnipresent within chemistry, although this is hardly made apparent to the wider audience.

Let's first consider the notion of validity in a chemistry context. Although chemical symbolism allows the application of well defined syntactic and semantic rules, neither the symbolical, nor the non-symbolical part of chemistry does translate into a strictly mathematical representation (Jacob 2001: 31–50). As a consequence, chemical symbolism is not just a syntactic, axiomatically driven combination of symbols, but also requires a semantic 'meaning' in the world of compounds that clearly escapes the kind of strict rationalisation and predictability available in mathematics and many areas of physics. Every synthetic chemist will confirm this, having encountered the pain of theoretically promising, yet practically unsuccessful synthetic pathways. On the other hand, the non-symbolic part of chemistry, i.e. interpretations, discussions and conclusions, mostly relies on arguments to the best possible explanation.

As a consequence, the kind of precision frequently found in physics and physical chemistry is not available to the many areas of chemistry where *interpretation* and *discussion* of results takes place. Whenever chemists make statements¹, provide explanations, develop arguments and draw conclusions they also, although not exclusively, act according to *philosophical* rules. In order to be scientifically sound, an argument in chemistry must be based on *empirically true* premises but also represent a *logically valid* deduction leading to true conclusions. Philosophers have long accepted the importance of the non-experimental part of science.

The aim of reasoning is to find out from what we already know something that we do not know. Valid reasoning serves exactly this function in science (...). A fundamental insight that the study of logic teaches us about reasoning is that we must distinguish the questions:

1. Are the statements in the argument true?
2. Is the connection between the assumptions and the conclusion a valid one? (Byerly 1973: 389–390)

The questions Byerly raises are highly significant for modern chemistry: generation of experimental data and generation of conclusions are both equally important. The interplay between empirical results on one hand, and sound reasoning on the other, forms the basis for chemical research. It is therefore not enough to just estimate the error range of the experimental results, but also necessary to discuss the validity of arguments based on these results. This brings philosophy back into play, this time in a more visible manner.

The following section of this paper discusses the logic behind arguments that are commonly used in chemistry. The third section briefly considers what happens when this logic goes wrong. The fourth section discusses the implications of these findings for our

¹ The term 'statement' is used here in its widest sense. It includes the outcome of non-experimental operations in chemistry, i.e. arguments, discussions, conclusions, models, hypotheses, theories, linguistic terms and expressions and also chemical symbols and reaction equations.

deeper understanding of how chemistry works as a science. The fifth and final section provides a brief summary and outlook.

The logic behind scientific arguments

A chemical text is a piece of (scientific) writing and, like any other text, is open to interpretation. It is possible to look at such a text from many different angles. For example, we can consider the text's grammatical structure, analyse the length of its sentences, discuss its aesthetic appeal or determine the logic behind its arguments. The fact that this is hardly done in practice merely points to the lack of interest in such an exercise, but not to the impossibility of such a task. Admittedly, who would want to scrutinise the syntax of a particular biochemical publication?²

A look at modern chemical literature is, however, highly instructive. Most arguments rely on an interplay of *Modus Ponens*, *Modus Tollens* and *Disjunctive Syllogism*, a result of the widespread use of conditional, causal hypotheses, negative controls and indirect reasoning.

The application of the *Modus Ponens* is particularly revealing (Table 1, p. 41). Deduction of a singular, empirically testable event from a general hypothesis is essential for any experimental science. If the experimental prediction is confirmed in the laboratory, the hypothesis is corroborated. It is not, of course, verified, since this would require the validity of the logical *Fallacy of affirming the consequent*. This is in line with both formal logic and Popper's notion of falsification. For example, if the two premises "all aqueous solutions of copper(II) salts are blue" and "this is an aqueous solution of a copper(II) salt" are used, we can predict that "this solution is blue". The latter can then be tested in an experiment. If the experiment shows that the solution is indeed blue, we can use this as corroboration.

² Text analysis is, of course, very common within literature, history, religion and philosophy.

ration of “all aqueous solutions of copper(II) salts are blue”, but not as verification.

If, however, a contradiction between theoretically predicted and experimentally found results is obtained, rejection of a hypothesis is possible. *Modus Tollens* and falsification provide the tools for this. For example, the experimental finding that “this solution is *not* blue” can be used to infer that “this is *not* an aqueous solution of a copper(II) salt” (*Modus Tollens*). Alternatively, we could use the theoretical prediction of a “blue solution” made by the *Modus Ponens*, combined with the two confirmed experimental findings that the solution is “not blue” and that “this is an aqueous solution of a copper(II) salt” to falsify the premise “all aqueous solutions of copper(II) salts are blue”.³

In practice, an experimental contradiction is frequently “explained” by uncertain experimental premise(s). This often results in extensive discussions. For example, the solution might not have contained copper(II) salts at all, but copper(I) salts, perhaps due to reduction; or the colour could have been masked or affected by ligands, pH or temperature. This allows chemists to question the experiment rather than reject their hypothesis. At this point, chemical reasoning departs from formal logic. Logical deduction of true conclusions from true premises is replaced by *ad hoc* explanations and the use of auxiliary hypotheses that try to justify the original hypothesis in the light of experimental counter-evidence. Ultimately, the question of what exactly constitutes ‘truth’ within chemistry, how we can assert it, and if it is essential for scientific progress, is raised (see also section four).

Another particularly interesting line of reasoning involves the *Disjunctive Syllogism* (Table 1, p. 41). Properly used, this allows chemists to use negative controls to indirectly deduce the presence of a particular entity or event by ruling out all alternative options. For example, if we know that a solution contains either copper or iron

³ In this case, the conclusion “blue solution” and the premise “all aqueous solutions of copper(II) salts are blue” are both false, and the premise “this is an aqueous solution of a copper(II) salt” is true.

salts, and we then find out that it does not contain copper salts, it must contain iron salts. To be successful, however, this logical syllogism requires the knowledge of all (reasonable) alternatives (i.e. no further salt alternatives, such as manganese or cobalt). In practice, this is frequently not possible and the *Disjunctive Syllogism* often fails because a particular alternative has not been considered. Again, this is a result of uncertain experimental premises. As a consequence, even if a logically valid syllogism is used, strict logical certainty cannot be obtained.

As we have seen, there are several fundamental problems with the use of logical syllogisms in chemistry. Deduction of logically valid conclusions frequently fails because the truth of the premises is in doubt or not all relevant entries are known. These problems occur even if logic is properly used. Not surprisingly, cases in which the chemical argument runs contrary to formal logic are even more problematic. The next section will briefly consider a few interesting cases where flawed arguments have been used in the past.

Table 1. Commonly used logical rules of inference. Please note that a contradiction between a deduced conclusion and experimental findings can be used to either reject Premise 1 or Premise 2 (or both) or might lead to the use of *ad hoc* hypotheses. $s \supset p$ reads 'from s follows p '; $\sim p$ reads 'not p '; $s \vee p$ reads ' s or p '.

Rule	Premise 1	Premise 2	Conclusion
Modus Ponens	$s \supset p$	s	p
Modus Tollens	$s \supset p$	$\sim p$	$\sim s$
Disjunctive Syllogism	$s \vee p$	$\sim s$	p
Fallacy of denying the antecedent	$s \supset p$	$\sim s$	$\sim p$
Fallacy of affirming the consequent	$s \supset p$	p	s

The logic of flawed arguments

This section analyses a few selected chemical arguments that have been made in the literature, looking at these chemical statements from the perspective of logic. This is a very unusual way to read everyday chemical texts, but, as we will see, it is rather instructive. The first statement from an undergraduate chemistry textbook describes the Jahn-Teller effect. The latter allows chemists to rationalise the shape of certain molecules.

If the ground electronic configuration of a nonlinear molecule is degenerate, then the molecule will distort so as to remove the degeneracy and achieve a lower energy. (Shriver et al. 1998: 255)

The statement above is given in form of an “if premise [P1], then conclusion [C1]” conditional line of reasoning.

From “the ground electronic configuration of a nonlinear molecule is degenerate” [P1]

follows “the molecule will distort” [C1]

The way the Jahn-Teller effect is explained here is problematic since it implies that the condition [P1] has to be fulfilled before the conclusion is true [C1]. Chemically speaking, this is clearly not the case. The molecules in question *are* distorted and do not contain a degenerate ground electronic configuration. The ‘if’ part [P1] cannot be fulfilled since the ‘pre-distortion’ form of these molecules does not exist — it is false. The conclusion [C1] merely describes the way such molecules are found in practice.

Paradoxically, this is not necessarily a logical problem since a true *as well as* a false consequent (conclusion) can follow from a false antecedent (condition) (Byerly 1973: 148). The argument is saved, logically speaking, by taking the form $[C1] \supset ((P1) \supset [C1])$, i.e. by following one of the paradoxes of formal logic.⁴

⁴ In short, the original, true consequent now becomes the true antecedent of the paradox.

It is odd, however, why the statement describing the Jahn-Teller effect should be based on a logical paradox. The chemical problem with this definition is highlighted by the implication of a time-dependent process where, if the ground state *is* degenerate, *then* the molecule *will* distort.

This can cause severe misunderstandings. When twenty-six second and third year chemistry undergraduate students at the University of Exeter were asked to comment on the meaning of Shriver's description of the Jahn-Teller distortion, *all of the students* discussed a process in which distortion occurs in order to remove degeneracy of the ground electronic configuration. For example (2nd year student): "The explanation of the mechanism of the process by which degeneracy is removed is lacking, however, overall the statement is understandable and clear as to what the molecule does in a given set of circumstances." The notion of a process might be a good illustration of the effect but is chemically wrong. All of the students questioned had at least partially misunderstood the precise meaning of Shriver's statement.

What is interesting about Shriver's logical construct is, however, that it allows him to bring [P1] into play in the first instance. By using a true conclusion [C1], it is possible to introduce a false condition [P1] without committing a logical fallacy. A similar approach to bring untested notions into play is based on logical *Addition*. If *q* is true, then *q or r* is also true, regardless if *r* is true or false. If *Addition* is paired with the *Disjunctive Syllogism*, a dangerous logical construct can result. Such a line of reasoning has, for example, been at the heart of the claimed discovery of 'cold fusion'.

Nuclear fusion reactions, such as the fusion of two deuterium atoms (²D) to helium (³He), release neutrons and consequently γ -rays. Nuclear fusion usually requires high activation energies and therefore has previously only been observed under extreme conditions (e.g. in the sun, during an atomic explosion). In 1989, however, the electrochemists M. Fleischmann and S. Pons conducted a number of 'cold' electrolysis reactions involving ²D₂O solutions and palladium electrodes at room temperature. During these experiments they observed an unexpected amount of energy that was released from the reaction vessels (sometimes even the explosion of the electrolysis

apparatus). They also detected the presence of γ -rays during these experiments. Based on these findings, they published a paper that postulated the occurrence of a nuclear fusion reaction (between two ^2D nuclei) during the electrolysis experiment.

While there are numerous problems with this discovery (e.g. experimental flaws, wrong conclusions), closer examination of one particular line of reasoning is highly instructive.

Use of eqn. (2) then indicates that reaction (v) takes place to the extent of $1-2 \times 10^4$ atoms s^{-1} (...). On the other hand, the data on enthalpy generation would require rates for reactions (v) and (vi) in the range $10^{11} - 10^{14}$ atoms s^{-1} . It is evident that reactions (v) and (vi) are only a small part of the overall reaction scheme and that other nuclear processes must be involved. (...) The bulk of energy release is due to an hitherto unknown nuclear process or processes (presumably again due to deuterons). (Fleischmann and Pons 1989: 301-308)



The authors have used the following line of argument:

From "data on enthalpy generation (of a normal nuclear process)" [P2]

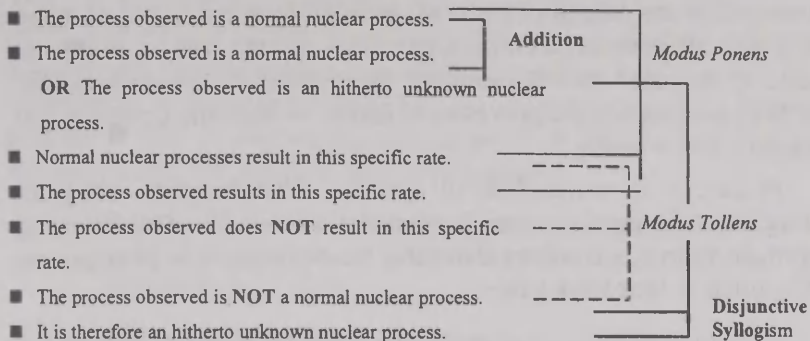
follows "rates for reactions (v) and (vi) in the range $10^{11} - 10^{14}$ atoms s^{-1} " [C2];

experimentally found was "(v) takes place to the extent of $1 - 2 \times 10^4$ atoms s^{-1} " [\sim C2];

therefore "bulk of energy release is due to an hitherto unknown nuclear process" [P2']

From a logical point of view, the authors have used knowledge about normal nuclear fusion reactions, together with experimental data [P2] to predict the reaction rates [C2]. Since the experimental data was not in line with these predictions [\sim C2], the authors should have concluded that either their experimental data was wrong, or that there was no nuclear reaction in the first instance ([\sim P2], *Modus Tollens*).

Instead, they introduce “an hitherto unknown nuclear process” [P2'] as explanation, using an experimental contradiction to introduce and verify an additional process not previously mentioned in the argument. This argument runs along the following lines:



This scheme illustrates the problems with the argument for the hitherto unknown process of ‘cold fusion’. In a logically correct world (normal and dashed lines), *Modus Ponens* is used to predict a specific experimental outcome, and *Modus Tollens* is used to reject a notion based on an unexpected, negative experimental result. In the logically flawed world (bold lines), *Addition* is used to introduce an hitherto unknown process, and, once *Modus Tollens* has been used to reject the normal process, the *Disjunctive Syllogism* then leads to the confirmation of the hitherto unknown process. Although all syllogisms used in the flawed world are valid, the problem arises from the use of the *Disjunctive Syllogism*.

Firstly, the *OR* statement “The process observed is a normal nuclear process. *OR* The process observed is an hitherto unknown nuclear process.” is only true, if one of its parts is true. In the cold fusion case, the truth of the *OR* statement above is therefore not determined. Assuming the second part remains hitherto unknown, then the first part initially has to be true in order to make the overall *OR* statement true. Interestingly, this part is later, when the *Disjunctive Syllogism* is used, required to be false. Changing the truth value of

this first part is obviously not allowed, and this also disallows the use of an *Addition/Disjunctive Syllogism* combination to introduce an unproven notion 'on the back' of a known one and then prove the unproven one by ruling out the original notion.

Secondly, if there are only two alternatives, and the first one is wrong, then the second one is confirmed. If there are, however, more than two alternatives, then *all* alternatives *but* the one to be proven have to be ruled out. By limiting the number of alternatives, the authors seemingly have proven cold fusion — logically correctly, but scientifically wrongly.⁵

Finally, it is worthwhile to consider what happens when incomplete arguments are used in chemical discussions. The following example from biochemistry illustrates the consequences of appealing to implicit or tacit knowledge.

An argument (...) in which one of the statements of the full argument is omitted, is called an *enthymeme*. (...) The power of arguments to persuade, especially in oratory, depends in part on leading an audience to fill in enthymemes for their common presuppositions. (...) A suppressed premise may or may not be true, and it may or may not be plausible. The task we set ourselves in this section is to find the categorical statement (if one exists) that completes a valid syllogism. (Byerly 1973: 129)

Jiang *et al.* have recently described experiments indicating that the compound ATP binds to the protein metallothionein and induces changes in the protein's structure (Jiang *et al.* 1998: 9146–9149).⁶ Since an experimental "Re-evaluation of the binding of ATP to metallothionein" by other scientists has already taken place (Zangger *et al.* 2000: 7534–7538) this example is particularly well suited for the discussion of enthymemes.

⁵ Independent investigations of this phenomenon have later shown that the experimental data could also be explained by non-nuclear electrode reactions (Petrasso *et al.* 1989: 667–669).

⁶ It is not the intention to criticise the experimental aspects or question the scientific value of this work. The aim is to analyse *formal* aspects of the arguments involved and to suggest possible improvements.

The observation that ATP enhances zinc transfer from MT to apo-SDH indicates that ATP changes the conformation of MT presumably to bring about more efficient zinc transfer. (Jiang et al. 1998: 9146–9149)

The statement contains one major line of argumentation with premise [P3] based on zinc transfer experiments from metallothionein (MT) to apo-Sorbitol Dehydrogenase (apo-SDH, an enzyme requiring zinc for its activity) in the absence and presence of ATP. This experimental premise is used to support the conclusion [C3] that the structure of metallothionein has changed upon ATP binding.

From “ATP enhances zinc transfer from metallothionein to apo-SDH” [P3] follows “ATP changes the conformation of metallothionein” [C3]

This argument obviously lacks further premises in order to present a full argument. This in itself is not a problem (it is impossible to go back to ‘first principles’ on everything) and the enthymeme can easily be completed by *explicit* introduction of the apparently *implicitly* used biochemical rule [P3’]. “In cases, where an enhanced zinc transfer from metallothionein to apo-SDH is observed, a change in metallothionein structure is involved.” Thus [P3’] would justify “enhanced zinc transfer to apo-SDH” as an indicator system for structural change of metallothionein via a *Modus Ponens* type inference.

Explicitly stating [P3’] completes the previously logically incomplete argument. Unfortunately, [P3’] is not really a widely accepted law or is supported by sufficient independent experimental evidence. On the contrary, enhanced zinc transfer from metallothionein has also been related to a number of events by the same authors, among them thiol oxidation and chelating effects (Maret 1998: 3478–3482).

It should be noted in passing that the alternative premise “A change in metallothionein structure leads to enhanced zinc transfer from metallothionein to apo-SDH.” [P3’], where the logical positions of “change in structure” and “enhanced zinc transfer” have been reversed, *cannot* be used in this context: inferring that a “change of

structure" has occurred from the observation of "enhanced zinc transfer" would constitute the *Fallacy of affirming the consequent*.

The three examples discussed here have indicated that (1) the philosophical discipline of logic plays an important role in handling chemical arguments and (2) that these arguments cannot result in mathematical certainty. In some instances, e.g. when the truth of premises is put into question or incomplete premises are used as part of the *Disjunctive Syllogism*, even logical certainty of an argument's conclusion cannot be obtained.

This raises a wealth of questions. The following section will briefly consider the implications for chemists' understanding of 'scientifically true' or 'false' statements.

Truth Versus Significance

The previous discussion has indicated that it is rather difficult to determine if a particular chemical or biochemical conclusion is true or false. Firstly, the kind of certainty provided by mathematics cannot be obtained because chemical symbolism is not the same as algebra. Secondly, chemistry heavily relies on arguments. The latter often involve inference rules that do not produce clear answers (e.g. *Fallacy of affirming the consequent*, *Disjunctive Syllogism*). Such arguments result in the most plausible conclusion, but not one that can be considered strictly logically valid. Thirdly, chemistry, as an empirical science, also relies heavily on experimental premises that might be true or false, depending on the skill of the experimenter. It is therefore possible that the truth value of the premises changes with time, and with it the truth of the conclusions — even if the syllogism used itself is logically sound.

Fourthly, there are serious practical difficulties in independently assessing the truth value of premises. While the early years of chemistry were characterised by scientists repeating each others' experiments to assess the data reported in manuscripts, modern chemistry is too specialised (and expensive) to allow for this kind of

independent assessment of experimental premises. *De facto*, most publications in the field of chemistry and biochemistry enter circulation without an independent check of the experiments.

Overall, it is therefore very difficult for a chemist to decide if conclusions drawn in a given chemical text are true or false. But, perhaps, this is not really the issue. This section considers possible alternatives to explain scientific progress, approaches that go beyond true statements, valid syllogisms, experimental testing and attempts of falsification. From the outset, it should be pointed out that the following contains thoughts and speculation that need to be supported by more evidence in the future.

Let's briefly consider how chemical journals classify a given manuscript once it is submitted for independent assessment.⁷ The reviewer is asked to judge the work according to the following criteria (taken from the Royal Society of Chemistry, Chemical Communications Referee Report Form, numbering added by C.J. for clarity).

[1] How would you rate this paper?*

Very significant*

Significant*

Routine

Scientifically unacceptable

* If you feel that the work reported is of sufficient significance to rank amongst the top 10% of papers published in ChemComm please indicate this.

[2] The experimental evidence supplied by the authors must support the results in the communication. Are the results in this manuscript supported by the experimental evidence supplied?

Yes

No

The referees are then asked to decide for or against publication and to justify their decision.

⁷ The notion of 'independent assessment' in modern chemical communication involves independent reviewers that are asked to comment on the overall quality of a given manuscript.

While there is an assessment to ensure the experiments are sound and the conclusions are properly drawn (number [2]), the category ultimately decisive for acceptance or rejection of such a manuscript is 'significance'. Using this category has many practical advantages. For example, it enables the rapid dissemination of scientifically novel and interesting work and prevents communication of routine work or possible repeats. From a philosophical perspective, the 'significance' criterion used by this and most other journals is rather interesting, since it might lead to an understanding of chemistry that is no longer exclusively based on true or false conclusions. Using 'significance' as the hallmark of chemical communication turns chemistry into an evolutionary process stimulated by significant discoveries. This resembles Lakatos' positive and negative problem shifts, with one major difference: the significant results might no longer have to be true. They might, in extreme cases, even be false. Nevertheless, it also avoids a slide into the kind of anarchy that Feyerabend's "Anything goes" might lead to. Clearly, not anything goes, but only the significant results do!

Within this pragmatic model, it might no longer matter if cold fusion was indeed 'discovered' in 1989 or not. Its postulation in that year was clearly significant and has stimulated research ever since. It was therefore perhaps useful for chemistry to have drawn this false conclusion, since it has stimulated new research.

The use of the 'significance', rather than the 'truth' criterion to describe chemical research has many implications for chemists and philosophers alike. Most of these issues warrant further reflection and cannot be addressed here. It is, however, worthwhile to point out two issues resulting from the use of the significance criterion: Firstly, significant, as well as insignificant texts can be true or false. It would therefore be interesting to find out which of these four possible scenarios, i.e. significant true, insignificant true, significant false and insignificant false texts, are most valuable to chemistry — and why. Do both kinds of significant texts equally stimulate further research, while insignificant texts will largely be ignored, even if they are true?

Secondly, chemistry generates new substances *and* knowledge about these substances. This knowledge is stored in extensive data-

bases, such as Chemical Abstracts and the Beilstein database that go back well over one hundred years. While insignificant communications might therefore be ignored for the time being, they do not simply disappear or 'die out', but can be reactivated at any time. The evolutionary process in chemistry is therefore not only selective, but also cumulative. Furthermore, the significance value of such a given piece of chemistry can change. The implications of sudden changes in 'significance' are clearly not fully understood.

Final remarks

The previous sections have tried to explore some philosophical issues related to chemical statements, such as logical validity, truth of premises and questions of significance. This has shown that logic can help chemists to better understand how they draw conclusions, although there are several problems associated with this. For example, the concepts figuring in the propositions may be imprecise. The premises of arguments might be uncertain (e.g. hypothetical). Not all reasoning might be based on strict deductions, and guesses, speculation, intuition, implicit assumptions etc. might play an important role. In the future, it might therefore be worthwhile to consider explanations of scientific progress and progression that go beyond the assessment of true and false statements. The question of significance plays an increasingly important role in chemical research, and philosophy has been slow to address the implications that result from this pragmatic approach. If science is no longer required to be strictly true, what does this mean for the wider understanding of the scientific process? These fundamental questions at the philosophy/chemistry interface will have to be addressed in the future.

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What Models Can Do: A Study of the Use of the Concept of a Model in Biosensor Research

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1. Introduction: why models and why biosensors?

1.1 Why models? Nelson Goodman once pointed out that models are promiscuous in their meaning (Goodman 1968). Many philosophers have tried to grasp their true nature but no consensus has been reached so far. Models are regarded as analogous to the objects which are modelled, and they are also interpreted as mediators between data and theories: in the latter case views vary widely on the issue what this mediation amounts to. In any case, no one seems to doubt that a model is something which represents something else, and that it resembles this something in certain respects, and to some extent.

Often models are analysed in their relationship to scientific theories. Models are used either for interpretation of theories in terms of empirically given data, or for connecting data within the framework of pretheoretical generalisations and hypotheses.

For decades, semantic and structural theories of models have been prevailing. However, as a number of recent studies show, this mainstream approach has neglected many significant features of models as they are actually used in scientific practice. Sergio Sismondo is one of the philosophers who has invited us to pay more attention to the complexity of models:

Whereas theories, like local claims, can be true or false, models and simulations are typically seen in more pragmatic terms, being more or less useful, rather than more or less true. Scientific models and simulations are given the status of tools, as well as representations; they are objects, as well as ideas. They easily cross categories, such as “theory” and “experiment”, the bounds of which are otherwise well-established. And modeling and simulation sit uncomfortably in science both socially and epistemically, because of the boundaries they cross. (Sismondo 1999: 247)

Because of the specificity of each particular case where “boundaries are crossed”, the traditional rigid classifications of models at best serve a heuristic role in setting out one’s preliminary research agenda.

As my point of departure, I shall start from Uskali Mäki’s distinction between four kinds of uses of the notion of a model. According to Mäki, the term “model” is applied, first, to the type of design (e.g. the 1997 model of SAAB, the German model of industrial relations). Second, “model” may designate an exemplar: an object proposed or adopted for imitation (e.g. a model student, a person displaying clothes in fashion shows, etc — that is, someone between the ideal and the real). Third, “model” refers to scale models or replicas (e.g. architect’s design of a house presented as a miniature construction, three-dimensional depictions of the solar system in science museums). Fourth, a model of a theory could be any set of entities, or a structure, which satisfies the axioms of the theory. “Theory” denotes a formal uninterpreted system of axioms and deductively implied theorems (Mäki 2001). In traditional semantic theories of models, the term is used mainly in this last sense.

Models can be made of something material, but they may also be of linguistic type — conceptual as well as pictorial. Some models are abstract entities (theories) while some are very concrete (material scale models). Models are always *of* or *about* something. In addition, the aforementioned types of models can be divided into two large classes — descriptive (scale models, equations) and prescriptive (talking of a “model student” means setting some kind of a standard).

As to the relationship between theories and models, according to a widespread view theories aim towards a true account of a system, while models can be used for different purposes without any commitment to their truth. (For instance, we say: this is just a model! — meaning a preliminary vague image that may lead to a new theory.) Traditionally, the function of models has been seen as one of providing interpretations for abstract theories, serving as facilitating instruments of scientific cognition (heuristic devices, sources of inspiration, suggestions for new theoretical directions).

The main philosophical problem concerning models has been well formulated by Marx Wartofsky (1979): how can one thing represent another? Wartofsky appears to think that anything can serve as a model of anything else, there must only be *someone* who takes it to be a model of something — in some respect, and for some purpose. However, Roman Frigg (2002) claims that someone's intentions are not enough to make a model a representation of something. It is the procedure of physical design that turns something into a model (of something). The practical aspect of model construction and the aims that guide modelling procedures have not been analysed in the mainstream theories of models. Therefore, one may agree with those radical critics who claim that these theories cannot explain how models actually represent their objects.

In some sense, models are like maps — created by us with some specific intention, in particular circumstances, and regarded as resembling the territory which is mapped (modelled). In order to better understand the role of mapping and modelling in actual sciences, philosophy of science needs to take into account the pragmatic aspects of knowledge production: there is always an explanatory gap, a kind of indeterminacy, interpretive flexibility in the ways models are “modelling” and maps “mapping” their territories that leaves room for social or cultural factors. Therefore, as a research topic, models should be of special interest to those researchers who are inclined to analyse the cultural and social settings of science. Sismondo has characterised the wide spectrum of issues related to models, which await further analysis, as follows:

Models become a form of glue, simultaneously epistemic and social, that allows inquiry to go forward, by connecting the ideal and the material. To do that they need to make compromises: they must simultaneously look like theory — because they have to explain, predict, and give structure — and like practical knowledge — because they have to connect to real world features. (Sismondo 1999: 258)

In my study, I aim to analyse some epistemic issues concerning models in their relationship to practical, social and cultural aspects of modelling. At the first stage of my project, I carried out a case study on model construction in biochemistry. I analysed the published papers and conference presentations of a group of biosensor researchers at the University of Tartu, Estonia. Preliminary results were discussed with one of the leaders of this group, and a series of interviews is planned to be carried out in the near future. My first goal was to “detect” all the different ways the notion of a model has been applied by this group of scientists. In particular, I was interested in different aims associated with different applications of the term.

1.2 Why biosensors? The reasons why modelling is studied in the present work on the example of biosensors are in part “historical”. Namely, I studied chemistry myself at the University of Tartu as an undergraduate and I know the chemistry department and the community of Estonian chemists relatively well. But it is also important that the biosensors’ group at the University of Tartu is an innovative research unit. The group has successfully combined high-level theoretical research with practical tasks and even commercial outcome. As will be seen below, biosensors are widely applicable devices; at the same time, constructing such devices is a theoretically sophisticated process. This makes the present case especially interesting and informative from the philosophical point of view.

Biosensors are analytical devices incorporating a biologically active substance which is intimately associated or integrated with a physical-chemical transducer (transducing system). The sensor yields an electronic signal which is proportional to the concentration of a specific analyte, or a group of analytes. Thus the interpretation (mo-

delling) of the output signal enables a fast and precise characterisation of the material analysed. The area where biosensors are used as analytic tools is rapidly expanding: the uses of the sensors range from environmental monitoring (pollutants, e.g. phenols, pesticides), and medicine (glucose, urates, etc.) to food industries. Many researchers in the field have emphasised that the quality of the new methods of analysis has improved remarkably in the last few years. The main advantages of biosensors in comparison with traditional analytical methods are speed, low cost and the compactness of devices (the weight of the whole system is approximately 200–300 g).

For my research purposes I interviewed Dr Toonika Rincken, the leader of the biosensors' research group, who also provided me with the relevant articles and conference papers.

The authors whose research reports I analysed, applied the concept of a model in a number of different ways and to different types of objects — instruments, processes, theoretical settings and entities, ways of application, etc. In the published papers there was no definition of model as such — the tacit dimension of knowledge appears to be significant in this case. However, the interviews and seminar papers revealed that the concept of a model is often discussed by researchers. For example, in one of her seminar papers Rincken gives a very clear account of the concept of a model:

A model is an imitation of reality which emphasises the essential phenomena, ignoring those which are less relevant for the model constructor. (Rincken 2002)

This statement indicates clearly that the scientist is aware of the pragmatic aspects of models, since the distinction between more and less relevant phenomena is a decision to be made in particular circumstances and by someone with specific aims. However, this is not the end of the story yet: this picture of a model seems to be a prescriptive theoretical model of a “model” for biochemists, an ideal

to be followed. In actual research context the notion covers much more and varies from one particular use to another.¹

According to Rincken, a model should be constructed in such a way that knowledge obtained for one particular system would enable generalisations and applications in different circumstances.

Real data are always better, but as the model enables to predict various developments, and it is not always possible to carry out an experiment, so the model does the work; moreover, most classical theories have been reached via some model. (Rincken 2002)

This passage reveals that although models are central (perhaps they are even the most important element of research), they remain secondary as compared to the *real data* or the true picture (theory?). Thus, the model is an instrument, a mediator, a tool or a supplement.

In general, Rincken characterises her work, both in the papers and interviews, as modelling, model construction. However, the construction of models is seen by her only as something which leads to new knowledge — i.e., to something which is more valuable and certain than the model itself. Modelling is indispensable at the first stage of research, but the real aim is pure theoretical knowledge.

For example, according to Rincken, one of the most intriguing problems in the development of biosensors is the loss of possibly useful information in the course of the analysis, because the aspect of the interpretation of the output signal has not been explored by researchers as thoroughly as it deserves. In spite of sophisticated analytical systems, only a little fraction of potentially available information is taken into consideration, and this makes biosensor analysis less reliable than it could be. Much of the research in this field is pragmatically oriented towards creating some simple fool-

¹ Diversity in the application of the concept of a model does not necessarily mean inconsistency. And the aim of philosophical analysis is in no way to criticise the chemists' work; rather, such an analysis attempts to identify and explicate the complicated boundary crossings between the epistemic and the social, between theory and empirical data, between image and reality.

proof analytic devices which could be marketed successfully. Rincken, however, pays a lot of attention to the purely theoretical aspect: a good model would also promote theoretical progress. (As already said, her group aims both at technological innovation and theoretical development.)

In the next section, I shall discuss in more detail some examples of the various applications of the notion of a model in the published research papers of Rincken's group. By and large one may distinguish between the following types of use:

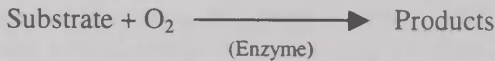
- models are *of* something: a model of an output signal; the signal itself as a model of the properties of the analyte; the biosensor as a model of sense organs, etc.
- models serve as guides for analysis: i.e. the model is an approach that involves certain methodological prescriptions for further research activities; certain values are kept in mind by the model constructor (such as simplicity and speed in this particular case, and of course, reliability which is the most important value);
- very often models are explicitly identical to formalised systems or even theories;
- models are more than just formalised systems; they also presuppose skills and expert knowledge in a broader cognitive area;
- models are objects for further analysis; as such they are something to be modified and improved.

2. The notion of a model in the biosensor case

A central research problem for the group has been related to the calibration of different biosensors. More complicated signal processing models such as the transient phase models require the determination of several parameters, which are not directly specific to the process under examination. In sociology of scientific knowledge, this type of problem has been called "the experimenters' regress" (Collins 1985). The essence of the problem is this: the greater the number of experimentally

determined parameters, the greater the indeterminacy and the need for further experimental tests of those parameters. In our case, the regress was stopped by the adoption of a new model.

One specific aim of the research was the construction of an enzyme-based amperometric biosensor. As a point of departure, two models of signal output — the exponential model and the integrated model — were studied and evaluated; as a result, a new approach to the problems of modelling the biosensor output signal and calibration was proposed. In this particular case, the signal modelling and calibration of the amperometric biosensor was based on oxidoreductases. Usually the enzyme-based amperometric biosensor consists of different oxygen sensors in combination with oxidoreductases, which consume molecular oxygen in the reaction of oxidation of a variety of compounds (Rinken 2000: 11).



The reaction dynamics can be monitored by the amperometric detection of O_2 or H_2O_2 . The biosensor generates a signal which is proportionally related, through some defined function, to the concentration of the measured analyte. The output signal depends on a number of factors, which have to do both with the biochemical processes and the characteristics of the electrochemical registering system. In principle, the output signal for biosensor calibration can be measured under conditions where the substrate transport and enzyme reaction have reached the *steady state*, or by measuring the *transient* (dynamic) phase of biosensor response (Rinken 2000: 12–13).

Both of these methods have certain shortcomings: one of them is relatively simple but slow; the other is rather complicated — it requires the measurement of many independent parameters, and it also involves sophisticated mathematics. The new model proposed by Rinken enables to

[D]escribe the biosensor output by means of a minimal possible number of parameters and allow the calculation of the final signal, corresponding to the steady state of the

process, from the transient phase of the response curve (*op.cit.* 14).

So, a model can do various things: it is a theoretical approach that describes something; it allows us to do some calculations; and obviously it is *about* something — it corresponds to something, is an analogue to a real process:

The models enable one to analyse, interpret, calibrate the signal. (Rinken 2000: 10)

This new approach integrates the advantages of both the steady-state and transient-phase measurements: it is fast, simple and reliable. Also, as seen above, the model has an interpretative and integrative function:

The better the model, the more information one is able to make sense of. (*op.cit.*)

One could find further examples of the “aboutness” of models. Thus, a model is applied to representations, or activities producing representations of something: it is the biosensor’s output signal that is being modelled (Rinken 2000: 10, 13, 14, etc.) — i.e. represented. At the same time, the signal is representing the analyte and its properties via another model. As Rinken says in her seminar paper (2002): “Biosensor is a system that makes the signal of the chemical reaction measurable and thus provides us with certain parameters of the substance analysed.” The model is capable of describing certain measurable parameters:

According to the model, parameters A and C are not independent, and for normalised data sets $A+C = 1$. (Rinken 2000: 21)

Either directly or via interpreted data the model is related to the part of reality being represented, even though it may need some additional procedures or calculations:

The biosensor output signal is characterised by an exponential dependence on time course. This model enables the calculation of steady-state parameters,

and:

this exponential model doesn't describe the very first part of the output signal.... so this kinetic model requires separate determination of the initial lag period of the biosensor and elimination of the initial data from the final calculations. (Rinken & Tenno 2001: 54)

Here, it is obvious that the group under consideration favours realist metaphysics. Such an attitude is not always so clearly present. Some model theorists, e.g. Frigg (2002), claim that a model can represent only another model as one does not have the access to the structure of reality as such.

Often models are taken to be a specific kind of abstract entities like a theoretical construction, or mathematical equation. Theoretical models have to be practically validated:

For the validation of the proposed models, biosensors with different parameters, containing glucose oxidase, tyrosinase and uricase, for the determination of glucose, catechol and uric acid respectively, were produced. (Rinken 2000: 15)

Thus (as will also be shown below), the models may be divided into theoretical and practical (sub)models. The concept of a mathematical model is applied on several occasions: Here is one example:

For many cases, the mathematical models are so complicated that they can be solved only by numerical simulation methods. (Rinken 2000: 14)

The model may even be directly identified with a particular equation:

According to the model (Eq. 16), the biosensor output depends exponentially on time and can be characterised by 3 parameters. (Rinken 2000: 21)

Equation 16:

$$Y(t) = \frac{[O_2]}{c_{O_2}^{\text{bulk}}} = A \exp(-Bt) + C$$

Models as abstract entities make use of the laws of nature — they are *like* theories, or *close* to theories. In this sense, the term “model” appears in the titles and subtitles of Rincken’s doctoral dissertation and articles. Frequently, in the published articles some section is called simply “Model”; in Rincken’s dissertation, a chapter is called “The models”. In this chapter, she suggests two new models (i.e., theoretical approaches) and provides application data. The sections are respectively called “The exponential model of biosensors” and “The integrated model of biosensors”. In both of these there are subsections called “Model applications (theory)” and “Model applications (practical)”.

On the one hand, the biosensor is modelled; on the other hand, the biosensor itself is a model:

The dynamic integrated model for amperometric biosensors, based on oxidoreductases, integrates the kinetics of ping-pong type enzymatic reaction and diffusion phenomena in the biosensor’s enzyme containing matrix with the dynamic lag of electrochemical diffusion-limited sensors. **This model describes perfectly the S-shaped sense organs and has been evaluated for glucose oxidase based biosensors as conventional model systems** but also for tyrosinase, uricase, and lactate oxidase based biosensors. (Rincken 2003: 1537)

And a theoretical model can be an object of another representing model:

[T]he oximeter-based biosensor can be seen as a model presenting the dependence of the oxygen concentration upon time and the substrate concentration in certain compartment. (Rincken et al. 1996: 861–62)

Different qualities can be attributed to models. Theoretical models can be reliable, simple or complicated:

Despite of uncomplicated experimental procedure, some steady-state biosensor models can be also rather complicated. (Rincken 2000: 14)

Models are taken to lead on to improved methods for calibration of biosensors:

A model of an oximeter-based two-substrate enzyme electrode is presented. The simplifications of the general model lead to a solution to different equations describing the influence of the rate of the enzyme reaction in combination with the diffusion phenomena on measurable oxygen flux. Both transient phase and steady state conditions for experimental data can be considered within the frames of the model and provide possibilities for the calibration of the biosensor. The optimal parameters for the biosensor calibration can be used in practical design of enzyme electrodes. (Rinken et al. 1996: 859)

Models also inspire and enable different developments (they have a heuristic function).

The modelling activities of the biosensors' group were guided by practical purposes:

The model characterises the influence of these processes on the experimentally measurable oxygen flux and can be used in practical design of enzyme electrodes. (Rinken et al. 1996: 861)

In this sense, models have to meet certain standards: models of biosensor output signal or calibration models (methods) are supposed to be simple, reliable and precise:

[R]elatively simple data processing procedures with a minimal amount of experimentally determined parameters ... This is an important condition to increase the reliability and precision of the analytic procedure. (Rinken et al. 1998: 801)²

Following Ronald Giere, one may characterise theoretical models as idealisations. In this sense, experimental data may deviate from the model (Rinken & Tenno 2001: 56), i.e. from the ideal conditions, or the norm.

² At the same time, the simplicity, precision and reliability would be achieved at cost of long time required for the measurement in the case of steady state measurements. The decision depends on the methodological values.

Rinken also speaks about *model systems*. The biosensors are sometimes called model systems:

More detailed discussion of constructing calibration plots and determination of lag periods for glucose oxidase based biosensors as **model systems** is given in (II). (Rinken 2000: 23, my emphasis — E.L.)

The concept of a model system deserves further investigation: for example, some philosophers have suggested that *theories* could be seen as model systems, or families of models (Hendry & Psillos 1999).

Rinken has also pointed out that the function and value of a model depend largely on the pragmatic context:

Depending on the aim and technical possibilities of analyses, one or another of the models can be exploited. The application of the proposed models gives a **profitable tool** for signal processing and calibration of various biosensors and the determination of concentrations of various compounds. (Rinken 2000: 28, my emphasis — E.L.)

To conclude this section, I bring one more quotation from Rinken where she concisely presents her understanding of what her model of biosensor can do:

The kinetic constants and activity of soluble and immobilised enzymes can be determined with a biosensor by applying the **dynamic integrated model**, which includes the inertia of the registering device, **for data management and calculations**. This **model of electrochemical diffusion-limited sensors** allows the **prediction** of steady state parameters for enzyme-catalysed reactions from a biosensor transient response and reproducible calculation of **real physico-chemical constants** without any additional experimental data. (Rinken 2003: 1535, my emphasis — E.L.)

As we see, the model allows the calculation of real constants, it enables data management and makes it possible to predict certain parameters. Models appear to have remarkable authority.

3. Concluding remarks

The case of the biosensor group shows the various aspects of models: they serve as interpretations of theories and represent real objects (processes, structures); they enable us to do various things; they have certain methodological authority and power of their own. The main purpose of modelling in this particular case is to obtain more effective, simple data processing procedures with a minimal number of experimentally determinable parameters for calibration. Simplicity, in its turn, is a necessary condition for the reliability of the analytical procedure. Simplicity, quickness and precision are the values one has to keep in mind when modelling. These values have to be seen in the context of a practical task: the practical aim of modelling was the construction of a device with given properties.

It seems obvious that a model cannot be simply reduced to some formula, or image, or description. There is a wide range of factors which influence and determine the content and meaning of a model. Context is very important: among other things, it includes the intentions of the researcher, the practical aims, resources available to the researcher (material constraints), etc. An abstract semantic theory of models would be unable to take into account all these aspects. Finally, there is a lot of ambiguity in the meaning of the term "model". Although researchers themselves switch easily from one meaning to another, without any serious misunderstanding, the different meanings should still be distinguished when speaking about models.

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Chemistry and Liberal Education in Partnership

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Introduction

A few years ago, the Nobel Laureate chemist Dudley Herschbach wrote: "Any chemist can attest to the usual reaction on being introduced to someone at a social occasion. Almost always they turn pale or wince, then refer to a mystifying college or high school course." (1996: 11) Herschbach believes that this infelicitous reaction of former students has to do with "the way we think and talk about molecules". Is it possible that something is missing, or is quite wrong, in our teaching of chemistry? We certainly need to be concerned about the image of chemistry, and about our ability to communicate our enthusiasm for this field. Chemistry should be more than "just a job", it should be at least a long-term interest, following the suggestions of the eminent sociologist of the 19th century, Max Weber (1968: 613).

It is easy to identify interesting projects which deal with the current problems of our society and culture, as long as we think primarily about the material side of life. Johnson's book "Chemistry in Context" (1994) contains a number of interesting case studies along these lines, dealing with foodstuffs, modern materials, energy problems, medicine, etc. And so does the somewhat dated "Opportunities in Chemistry", written under the chairmanship of George C. Pimentel (1985). In this essay we will deal with chemistry in a much wider context, defined by its relationship to, ultimately, the *values*,

meanings and purposes of life, and to *human interests*. These are all topics which are usually considered in liberal education courses (Schneider 1999, Cronon 1999).

This material is also frequently of interest to all who study general aspects of the elusive philosophy of chemistry. We will thus want to see whether liberal education can at times serve as a stand-in for this latter discipline. We are not aware of other very similar “experiments”.

There are many attempts to interest young people in chemistry by offering demonstrations: for example, the apparent transformation of base metals into gold, color changes of indicators, clock reactions, miniature volcanoes, “barking dog” reactions, etc. All this is fun — but can these demonstrations help young people to experience the satisfaction that comes with having a part in true discoveries, in things that really matter? Also, would these activities help to improve the image of chemistry in the long run (an image, which has already suffered unjustifiably for other reasons), and to keep former students from having bad memories, forever?

Given the overall motivation for this study, we need to outline our approach. In the first part we will discuss some fairly simple ways of integrating matters of human interest into the teaching of basic chemistry. Next, we will turn to a more advanced topic, the “molecular structure conundrum”, centering on the question whether molecular structures can and should be obtained with the help of quantum mechanics. This will lead us to concentrate on Niels Bohr’s out-of-the-ordinary philosophy. In the third part we will discuss several related topics, such as nonverbal communications in chemistry.

Liberal education opportunities in basic chemistry

Integrating notions of human interest into the teaching of chemistry may very well start at the basic level, provided the discourse of chemistry is cautiously widened. The negative comments of many

former students that Herschbach spoke about would hopefully no longer be heard, and the image of the field be enhanced.

On the positive side, most of the basic chemistry texts show great mastery of the subject matter and completeness. They tend to be colorful, easy and pleasant to read, and coherent. They also contain much helpful material, such as examples and self-tests. In a very good text, like that of Jones and Atkins (2000), the coverage is reasonable and well balanced; it is obvious that much care was taken in this book's development.

On the downside, however, the material presented very often does not give a realistic picture of the immense effort the authors and countless others contributed to the project, directly or indirectly. The story told in the published text is perhaps *written too well* and everything seems to be well understood and definitely settled. As a result, the readings lack excitement. Most students probably would like to experience the suspense that was involved in the work, like what one would find in a good detective story. It need not describe "all the warts", but should still be true to life and ultimately lead to the satisfaction of a job well done.

Miller (1995) experimented with this "suspense factor" in teaching, where he traced, as it were, the step-by-step developments in a research project, even including (within reason) the detours, misconceptions, and other errors the authors had to overcome before reaching their goals. The student interest in all this was high.

Along similar lines, Derek Davenport (1993) carried out an interesting pedagogical experiment: he found that students very much preferred to study journal articles written about 200 years ago, where the authors let the readers know the soul-searching and the agony they had to endure, in trying to make sense out of what they saw and measured in the laboratory. This contrasted favorably with the smooth, perhaps smug, contemporary literature, where everything seemed to be certain and free from suspense, and which all too often left them cold.

In addition to outright suspense, student enthusiasm can certainly benefit from all manner of "human interests" in the context of liberal education, as has been done in a masterful way by the Nobel Laureate

chemist Roald Hoffmann, especially in one of his books "The Same and not the Same" (1995). Of course there are few *direct* and close connections between the two disciplines, and we will now illustrate what we mean by *directness*.

Hoffmann writes: "What do you want when you come to the physician with your aging father, who is weak and feverish? *Compassion* to be sure, but also a workup of blood chemistry or a test for the organism possibly causing the suggested pneumonia." (1995: xiii)

Herschbach, whom we mentioned earlier before and who showed much interest in experimenting with novel pedagogical methods, gives another example. When talking about routine student exercises, he says: "The usual textbook problems should bear a warning label "*Too much of this stuff is dangerous to your mental health*", because the excessive use of such exercises might lead to impassivity relative to this academic field."

A third example is the age determinations carried out on the Turin Shroud, claimed to be the burial shroud of Christ. Many Christians would take an age determined to be about 2000 years as proof of important parts of the New Testament's message (Warner 1989: 101A).

Far more typical than the above links are the indirect connecting points between the disciplines we are considering. A very impressive example is found in the textbook of Jones and Atkins (2000: 362). It is based on a very unusual photograph of mountaineers camping next to a vertical wall of rock on Baffin Island, their tents being suspended far above the level ground, using high strength ropes. The reader is certainly able to grasp the important technical point of this picture, that is the immense strength of the suspension cables manufactured from high tensile strength polymers. In addition, the viewer is made aware of his or her own self-preservation drive — but that is where it ends. There are a number of conceptual connections to the *values, meanings and purposes* of our culture, which are part and parcel of the liberal educational subject matter that may come to mind. For example, one might think about the ethics of reliable quality control work, the possibility that tents, once they break loose, are likely to

hurt others below, or the aesthetic pleasure of seeing the scenery from a very unusual vantage point.

At times it is very easy to decide whether a given value, meaning or purpose is or is not likely to be of interest to students in chemistry or liberal education courses. For example, Jones and Atkins (2000: 362) discuss the “perception, thinking, and learning, which depend on the shapes of molecules...”. Here at least a few words like “amongst other things” could be added, for factual and philosophical accuracy. One or two literature references would definitely be in place, under “Further Reading”, such as to the article “Must a Molecule Have a Shape?” (Woolley 1988: 33) and “Molecular Shape, Reduction, Explanation, and Approximate Concepts” (Ramsey 1997: 232). Very little space and time are needed to introduce, or to read, such small additions. On the other hand, leaving aside these interesting minor comments or questions means losing opportunities to contribute to the overall topic. The (still) strong *positivist* orientation of many chemists, both of authors and of readers alike, may very well be the real obstacle in this situation.

A more involved situation is the following: Jones and Atkins at one point discuss “what it means to be conscious” (2000: 362). This cryptic and short statement does not help; it is miles from the very thoughtful and informative discussion of the eminent physicist A. B. Pippard (1988) who is convinced that “consciousness” is out of reach for the sciences, at least at this time. If consciousness is to be related to molecular shape, as Jones and Atkins hope to do, it should be presented with at least a few more words of explanation, plus a few well-chosen references, to indicate the depth of the waters one is about to swim in. The price for the omission is high in this case: valuable stimulation of the student interests is lost by the oversimplified approach.

In summary, the liberal education opportunities discussed thus far are eclectic but they are not very coherent, and allusions to human values and purposes found in the textbook literature tend to be indirect and far-fetched. To find more interesting examples we must dig deeper.

The “molecular structure conundrum”

Our first example of this sort deals with the central concept of molecular structure. Surprisingly, this conundrum or riddle has persisted for a long time, and, which is worse, it is all too often passed over in silence.

Very briefly, the conundrum lies in that classical molecular structure, derived from various experimental data and classical theory without recourse to quantum theory, is well established and is immensely useful, but there is a serious open question “whether classical molecular structure can, will, or should be derived from quantum mechanics” (Weininger 1984, Woolley 1985).

Weininger realizes that in the literature one finds a wide range of answers to the above question, which however fall into three fairly distinct groups. A first group of workers, including R. F. W. Bader (1980, 1994), believes that one can indeed account for the classical molecular structure, if one uses what is called “subsystem quantum mechanics”. Here the molecular average for a given property is taken to arise as the sum of atomic contributions. The additivity scheme so defined, whether it be based on atoms or groups of atoms as building blocks, requires that the atoms be at least “*essentially*” transferable between molecules, a condition which tends to be satisfied for molecules of similar structures (Bader 1990: 2). More recent results caused Bader and his coworkers to look forward “to increase the effectiveness of the functional group concept through the replacement of the present qualitative and largely empirically derived knowledge of group properties by the predictions of quantum mechanics” but they realize that further advances in subsystem quantum mechanics are needed “to put physics to its fullest use in chemistry” (Bader 1994: 2). It is an open question whether this “fullest use” leads to a much higher transferability in most cases tested or whether exact solutions of the subsystem quantum mechanical calculations are needed.

In contrast to the first group, Weininger’s second group is exemplified by Woolley (1985), Primas (1982) and other scholars

who deny that molecular structure can be obtained by quantum mechanics, and that the logical structures of quantum and classical theories prevent a scientist from deriving each one from the other. The treatment relies heavily on the complementarity principle, which will be discussed shortly.

The third group of Weininger consists of workers who believe there is a basic flaw in quantum theory as it stands in that it is incomplete and involves hidden (i.e. non-observable or non-measurable) variables. David Bohm is the most prominent representative of this group. At the present time, it is known that hidden variable theories can in fact be constructed, but that a high price must be paid for doing so, discussed in some detail by Bell (see Primas 1983: 109–111). Conversely, an intriguing interpretation can be found for Bohm's theory which relates the appearance and the decay of several types of order, the meaning of dialogue, the concept of truth beyond reality, etc.¹ Bohm's theory is observationally equivalent to the commonly accepted Copenhagen version, and Cushing (1994: 174–186) has thought of a counterfactual scenario, which in the crucial decade of the twenties could have led to the acceptance of the Bohm theory, in preference to the Copenhagen interpretation. As an aside, Herbert (1985: 17) claims there are at least 8 different interpretations of quantum mechanics, all based on the Schroedinger equation and thus on the Copenhagen approach. In the minds of a minority, Bohm's theory remains a viable alternative to the Copenhagen version of quantum mechanics (for example, see Kronz 1999). Philosophers generally seem to be preoccupied with finer points of their trade, and the worldviews relating to different interpretations are not always given much attention.

Liberal education would probably delve into the question whether both worldviews (or others) are in fact reasonable and acceptable (see many-world theories for details). We think they are not.

¹ The eminent physicist Cushing considers a theory to consist of an explanation, i.e. a formalism, followed by an *interpretation*, which is the "story" that enables us to fully absorb or understand the theory (1994: 11).

The epochal work of Niels Bohr

We are now returning to the second group of Weininger, since there are, aside from the question of a “best” worldview, some interesting links between liberal education interests and our molecular structure problem. This philosophy was remarkably productive in microphysics (Honner 1987). We will be concentrating on the central concept of “complementarity” which Bohr suggested in 1927 to account for “situations where two different conditions of observations yield conclusions that are conceptually incompatible” (Primas 1983: 349). Bohr’s philosophy has led to very diverse comments, such as “Niels Bohr is regarded by many as a heroic visionary of twentieth century physics”, and by others as “an obfuscating mystic” (quotes collected by Wise 1987: 411).

The principle encourages the invention of new “contexts”, complementary to those already known. Old and new concepts together will lead to a full description of an atomic system. Here “context” is a “complex set of rules that enable us to interact with nature, [and] they define a point of view” (Primas 1983: 325). Also, “[t]here are many possible forms of truth which are mutually incompatible but not contradictory since they can be interconnected by dialectical thinking” (Primas 1983: 326).

The term “dialectic” has a long history; it was used by Kant to describe arguments, which show that “principles of science have contradictory aspects” (Honderich 1995: 198).

Bohr excelled in acknowledging the contradictory parts of experience, without trying to reduce them to one another. He also tended to sustain, rather than resolve, the sharp dialectic tension between opposites, such as the inevitability of classical concepts for an inherently non-classical world (Beller 1992: 178). Also, Bohr was quite able to use a dialectical mode of synthesizing, rather than rejecting opposing views (Beller 1992: 151). Undoubtedly, this willingness to synthesize by dialectical methods contributed much to the success of his philosophy of complementarity.

The Copenhagen interpretation Niels Bohr and others developed is very much the product of Bohr's "superhuman" intuition. His philosophy is not "proven", or obtained by analysis, but it is based on the complementarity principle, which has generally been accepted in modern quantum theory (Honner 1987).²

The all-important notion of complementarity certainly defies ordinary experience, in that we are expected to hold two concepts together, which are mutually exclusive, shattering our usual framework (Honner 1987: 102). Nevertheless, we want to clarify, if possible, how this notion can be a rational generalization of causality, as Bohr insists, time and again. Following Honner (1987: 56), we agree that cause and effect are normally or classically seen as part of a sequential network of processes or events, but complementarity, considered as a rational generalization of causality is somehow a circular (or "more circular") account. Forward and backward paths of some process may follow different paths, and thus approach a circular path or one of several variations of it. Paths or events may thus become intertwined (Honner 1987: 56).

Another generalization of occasional interest to us is the 2-layer structure of language which Bohr used, but here the layers are intertwined (Honner 1987: 221). For future reference we note here that dialectic thinking involves one further generalization, that is the possible repetition of events.

Honner, who studied Bohr's work very carefully, also stated: "Philosophically, ... Bohr's case [i.e. his theory] is reasonable. And, from the point of view of physics, his case has its firm warrant until either quantum theory is overthrown or is radically altered." (Honner 1987: 220) There are a number of scholars who believe that Bohr was clearly affected by his cultural, personal, professional, and cognitive milieu and by various psychosocial factors, such as ambition, professional interest, and group dynamics (Beller 1992: 177 and 179).

² Very accessible discussions of the complementarity principle are found in (Honner 1987) and (Wick 1995). Our presentation concentrates on the philosophical aspects, not on the algebraic formalism, which is discussed for example in (Primas 1983).

Probably these influences merged and, in Beller's words: "[T]ogether they served as fuel for Bohr's passion for science and gave meaning to Bohr's spiritual life."

On thinking about this, we find that we can discern ever more clearly a bridge from chemistry and physics to liberal education — the *values, meaning, and purposes of life*, which we mentioned earlier. For one, many (sets of) complementary views have been suggested in the recent decades, not only by Bohr, but also for example by Primas who said: "Science, art, religion and moral philosophy do neither conflict nor have they to say nothing to each other, they rather represent complementary aspects of the same reality." (1982: 293, and especially 299) Primas and Honner listed a number of areas of work, which can probably be related by complementary thinking: mechanics vs. thermodynamics, Newtonian vs. Einsteinian mechanics, physics vs. chemistry, and structure vs. function (Primas 1983: 349, Honner 1987: 57).

Secondly, Bohr and his colleagues were deeply involved in the birth of modern microphysics, not only in their thinking, but emotionally as well. As a result it has been noted: "Nearly every physicist has his own Bohr. Each re-translates Bohr into his or her own intellectual environment." (Kaiser 1992: 237) People certainly admired Bohr for his outstanding intuition, but in many cases they also disagreed with him sharply (see the detailed description of the exchanges of Bohr with many of his colleagues; Beller 1992: 147).

As a result of these things, Wick asked: "What special attributes of personality or philosophical outlook are required for an otherwise respectable scientist to put forth a theory utterly lacking a rational foundation?" (1995: 11)

The outstanding intuition of Bohr is part of the answer; we immediately recognize that this relates to both, a person's "people skills" and to his or her ability to deal with human nature as well as to his or her scientific stature. The former aspect relates not only to a person's interactions with others, but also to knowledge and comportment of self.

That much said, we realize that creative scientific work fosters and favors skills and attitudes of great interest and value in scholarship generally, and in liberal education in particular. We are moving, in fact, in the direction of a unity-of-scholarship.

A second part of our answer to Wick's question is simply "courage", and we wonder when such courage is justified. A bit of historical knowledge and human insight will tell us that the milieu, the general human climate is important here, factors which certainly affect the quality of communication and understanding. Again, we note a distinct bridge to *values, meanings, and purposes in life*.

Verbal and nonverbal chemical communication

We are alluding here to the need for iconic and symbolic languages, in addition to the vernacular (Grosholz and Hoffmann 2000).

Herschbach noted that much of the work of beginning chemistry students is similar to what they must go through when learning a foreign language (1996: 11). A researcher, however, may at times face situations where he or she has to invent a language, or an entire discourse, in order to communicate with "nature". Even mature scholars often struggle with language problems — at times they need to extend or overhaul the entire discourse they are familiar with when new and exciting results are obtained. Heisenberg used three different terms, in addition to "uncertainty", when he first tried to express the latter concept, in his pivotal paper; it was as if he wished to illustrate the concept of uncertainty semantically (Wick 1995: 35).

Chemists face a never-ending challenge, because the language barrier they deal with continually keeps growing, with every new set of reliable data, every new instrumental method, and every new concept that comes into usage.

At the bottom of this problem lies the simple fact that chemists, as Grosholz and Hoffmann put it, "live in two worlds, and must continually move back and forth between the two, the macroscopic

world of the laboratory, and the molecular world, invisible but powerful”.

There is an interesting analogy here, in that the discourse of classical physics becomes incomplete, and helpless, when the observer studies microphysics, unless some way of translating from one “world” to the other is found.

Since the region of overlap between chemistry and liberal education is limited, even non-verbal aspects of communication are important; they are more plentiful in chemistry than in many other sciences, anyway. For example, it has been said that “chemists think with their hands” (Kovac 1999: 1) and that “the true language of chemistry is to be found ... in its *praxis*” (Laszlo 1998: 69).

In spite of the looseness or flexibility, often necessary in the thought process, the languages one finds in published chemistry textbooks and journal articles are often quite rigid, and as Derek Davenport (1993: 32) put it, “introductory courses have all the flexibility of papal bulls”. Often this is intended to give the impression that the subject matter at hand represents objective knowledge, not just the opinion of one, or a few, authors. As Hoffmann puts it, the finished article “reports real facts, but at the same time it is unreal. It obscures the humanity of the process of creation and discovery in chemistry” (Hoffmann 1995: 63/4). He even talks about possible “real crimes against the humanity of the scientist” because he is expected to present a “sanitized, paradigmatic account of a chemical study, one that suppresses many of the truly creative acts”.³ Between these are the human mind and hands responding to the “chance happening”, the fortuitous circumstance — all of the elements of *serendipity*, of creative intuition at work (Hoffmann 1995: 61, 63–4). Sometimes the language is called “thought in action” (Grosholz and Hoffmann 2000: 245).

³ “Sanitized” language constitutes the final distillate, as it were, of a piece of work, and does not show remnants of the non-productive asides and errors a researcher had to overcome before arriving at his final conclusions. Hoffmann presents detailed information on the history and the severity of this problem (1995: 58).

There is an interesting contrast between Polanyi's theory of "tacit knowledge" (Brandt 2003) which says that "We know more than we can tell" and the idea presented here, which can be formulated as "We can tell (that is, *communicate somehow*) more than we know (that is, *know explicitly*)". One can think of this interaction as a dance of many partners, each being in touch and thus communicating with a few nearest neighbors (Gelwick 1977: 60). As a result, the entire group has a certain coherence, and multi-step communications travel back and forth, non-verbally. Polanyi's theory likewise can serve to explain non-verbal communications of numerous skills in chemistry and elsewhere. Along similar lines, von Weizsaecker (1980) studied "the unity of science as a function of human performance" and "in the still unanalyzed context of the essential interrelation of experienced man and experiencing nature".

In a similar vein, the integration, or "socialization", of a new worker into an existing research group has much to do with teaching a new terminology, and perhaps with the adjustment or bending of old terms, as described by Kuhn (Davenport, Edward 1990: 17).

Clearly, non-verbal communications appear in many guises and serve to broaden the discourse.

Desirable "guesswork"

From the last few sections we conclude that there is no hope that we might really arrive at a "complete" discourse (if that ever exists), unless we try to "cut nature at the joints" by identifying links between chemistry and other fields of work. This may be a tedious matter, though, and chemists are usually too pragmatic to wait for a more systematic approach.

In most chemical studies theory and practical matters form a thicket and both, beginning students and old researchers alike, may initially be at a loss as to how to handle a given problem they may be interested in, at their respective levels of interest. Herschbach, whom we met earlier, has given much thought to develop new and effective

pedagogical methods: he experimented with several techniques as he aimed at getting students to proffer guesses whenever there seemed to be no other way to get a first handle on a problem. He pointed out that even veteran research scientists may have to do so at times, but he added that “a genuine expert is also obliged to devise means to test the guesses” so that false guesses can be set aside early. In another situation, which ultimately led to a remarkable discovery, Hoffmann (1988: 182) found that progress was achieved by “a wonderful, chemical process of hints, analogies, facts and intuition” — a combination reminiscent of the alchemy of old.

One can find many examples in the history of science where guesses led to hard work and ultimately to valuable discoveries. Famous cases of this sort include Bohr’s struggle to formulate the complementarity principle in ever more understandable terms and David Bohm’s quantum mechanics mentioned earlier.

Returning to Hoffmann’s work, we note that this author has written about, and has utilized a number of ideas which could very well be presented in the framework of philosophy of science, or specifically of chemistry, and would be in place in liberal education as well: in recent years he published a number of articles dealing with the methods of research and teaching. In one of these, titled “Nearly Circular Reasoning” (1988: 182) he describes what he calls the “curious role of logic in science”: in a typical case he believes that the reasoning was based on a “soft theory”, defined as one that would probably be confirmed in 85% of subsequent trials. At times, when data are not quite conclusive, he says, chemists may be willing to base their thinking and planning on intuition or “jumps of the imagination”, on non-deductive arguments or on hunches, which may be notions of unknown or forgotten origin. At another point, Hoffmann talks about the reasoning as proceeding by the “crudest analogy, or by the primitive ideas that no one wants to admit to in print”.

Hoffmann and philosopher Immanuel Kant are examples of scholars who were both very open and honest in communicating what they knew to be valuable methods of research. They differ to some extent when they describe the driving forces at work in a person: Kant’s “mother wit” had to do with “...a secret trick that Nature

employs” (Webb 1988: 40) while Hoffmann believes the “awesome force of individual psychological conviction ... propels one to true innovation”. The “awesome force” reminds us of Polanyi’s “passion” (1958: 132–179) and the “psychological conviction”, a fairly general term, probably relates to Polanyi’s “tacit knowledge” (Brandt 2003: 333). As in earlier contexts, a scholar may benefit very much from his continual practice of “guessing well”, from staying connected to his “psychological conviction”, probably the result of his liberal education.

We are mentioning these items because we believe that Hoffmann’s willingness to show us the important tools of his trade is a great help to younger, less experienced scholars who are trying to solve difficult chemical problems. His teaching, in our view, represents liberal education at its best.

Concluding remarks

There are of course many possible entry points for a study of the sort reported here. One may consider the history of chemistry or some of the ethical questions arising in the laboratory, in teaching or research. Alternatively, one may wish to concentrate on the image of chemistry, an image which has suffered a great deal, undeservedly, in recent years.

Obviously we cannot go into these matters for lack of space, but we like to mention at least some additional ideas which might also strengthen the partnership of chemistry and liberal education.

First of all, liberal education is an important potential stand-in for the philosophy of chemistry, which has been slow in coming. Both fields deal with very general questions, they are co-extensive in many ways.

Secondly, chemistry is often considered a service science, for obvious reasons, and in various contexts. We want to suggest that liberal education courses are, or should be, a service at a high level.

They may well be a prelude, or an integral part of a number of very interesting and demanding special topics courses. Some examples of interesting analogies are as follows:

- the laws applying to various chemical particles, and to aggregates of huge numbers of the same types of particles, compared to the laws applicable to living organisms and their societies;
- complex events which involve repetitive or very similar processes and, simultaneously, unusual and quick changes (reactions or transport processes), again in comparison to living organisms (evolution and revolutions);
- the often imperceptible apparent violations of laws as evidenced by emergent properties, or less than perfect chemical communications. As an example, we consider especially the sharing of some intuitions or of uncertain knowledge. One particular class of intuitive arguments deserves special mention here, that which does not follow any rules. Earlier we discussed the work of Polanyi (Brandt 2003: 336–341) who noted a “fundamental inadequacy” in Kant’s thought. He said “... even a writer like Kant, so powerfully bent on strictly determining the rules of pure reason, occasionally admitted that into all acts of judgment, there enters, and must enter, a personal decision which cannot be accounted for by any rules” and “no system of rules can prescribe the procedure by which rules themselves are to be applied” (Webb 1988: 40). In the “Critique of Pure Reason”, Kant notes that what ultimately determines the application of rules is our “mother wit”, a “skill so deeply hidden in the human soul that we shall hardly guess the secret trick that Nature here employs” (quoted by Polanyi in Grene 1969: 105).

Polanyi felt that for Kant to admit this much means that he implicitly undermined his entire critical enterprise as he conceived it. We do not agree with this conclusion, since the openness, which Kant displayed, must have impressed his readers, thus causing them to obtain more benefits from his work. The development of his philosophy probably gained much from Kant’s ability to assess his own work objectively and unselfishly.

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The Logic of Place: Kitaro Nishida on Self-Consciousness

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I know that I exist; the question is,
what is this 'I' that I know?
René Descartes

Prologue

This paper was initially meant as an analysis of a current issue in philosophy of chemistry. Namely, it was my intention to consider the topic of natural kinds and essentialism in chemistry in terms of the philosophy of Kitaro Nishida whose ideas I briefly discussed in my presentation at the previous ISPC symposium (Hojo 2003).¹ Rom Harré is one of the authors who has examined this topic. In this connection, I was fortunate to come upon an exciting new book by Harré (2002) titled *Cognitive science: a philosophical introduction*. This book especially helped me to begin to perceive certain major differences between Nishida and other contemporary thinkers. In particular, it became clear that there is a tremendous gap between them concerning the concept of the self (or consciousness, or self-consciousness). Furthermore, I noticed that Nishida's most important

¹ I was inspired by Rein Vihalemm's paper (2003) "Natural Kinds, Explanation and Essentialism in Chemistry", which concerned arguments proposed by Rom Harré (2001) in his review of *Philosophy of Chemistry* by Jaap van Brakel (2000a). Related themes are also examined by van Brakel (2000b, 2003).

thought — the logic of place in consciousness — has not really been acknowledged neither in philosophy of science nor in cognitive science.² As this concept seemed to provide important hints for the most difficult problems in philosophy of mind, I decided to devote my paper to this aspect of Nishida's ideas.³

Psychology cannot do without the person

Rom Harré observes that “in psychology, materialism has been explicitly advocated in various forms and has been implicit in the presuppositions of research programs and proposals” (2002: 79). He then asks: “But why have ontological, methodological and conceptual materialisms been abandoned by many psychologists in favor of assumptions about the reality of cognitive process?” His answer is that “psychology cannot do without the person”.

Harré (2002: 89–90) clarifies the concept of a person as follows:

Kant ... called this the ‘transcendental unity of apperception’. It is not a thought, a feeling, an object of perception or an action, or any combination of these. It is a unity because for each person there is just one field of thoughts, feelings, perceptions and actions of which he or she is conscious. Persons are necessarily embodied. Persons are neither thoughts nor feelings, nor can they be perceived, nor are actions. They are the ontological basis of a scientific psychology, but they are neither material nor immaterial.

It is surprising to find that the notion of a person explicitly specified by Harré in the context of scientific psychology closely resembles the personhood which Kitaro Nishida described in his first book *An*

² Some of Nishida's earliest work has been mentioned in cognitive science studies (Osaka 2002: 26).

³ For problems on the self and consciousness, see, e.g., Chalmers (1995, 2002), Gallagher and Shear (1999), Varela and Shear (1999). For some views of scientists and religious thinkers on this issue see Barbour (2000: 122–149).

Inquiry into the Good, published in 1911 (CVN 1: 3–202).⁴ Many of Nishida's descriptions indicate that the unity of consciousness as described by him corresponds to the character of a person in the cognitive science model above (CVN 1: 142–168). However, his understanding of consciousness underwent various changes during his philosophical career. Nishida had struggled with the idea of self-consciousness for a long time before he arrived (in the middle phase of his work) at the idea of 'place'. His later views were all based on this idea. The tremendous difference between his initial view of 'pure experience' and his final view of 'action-intuition' (CVN 8: 541–671) seems to be reflected in the gap observed between his final philosophy and that of other contemporary thinkers. Therefore it is essential to see how he developed his idea.

The development of the idea of place

Nishida was deeply influenced by the philosophy of Henri Bergson (1859–1941). He tried to maintain Bergson's stance against Kantian philosophies, such as that of Heinrich Rickert (1863–1936), by gradually developing his standpoint from 'pure experience' to 'absolute will' as the most immediate reality. This shift was based on the idea of consciousness advocated by Johann Gottlieb Fichte (1762–1814). The shift in question was documented in Nishida's second major work, *Intuition and Reflection in Self-Consciousness* (1917) (CVN-2: 3–350). During this period, Nishida recognised that 'intuition' was at the base of absolute will — where there is one acting, there is one seeing.

Nishida became critical of the epistemology of the then popular Kantians and of the neo-Kantian school, which presupposed a conflict between the subject and the object, consciousness and its object, form

⁴ References to the collected works of Kitaro Nishida, 4th edition, published by Iwanami (1949) will be abbreviated as follows: CVN-volume number: page.

and material. In Kantian philosophy, knowledge was considered to result from an operation that unites the materials of consciousness given by perceptual intuition, and another operation that reconstructs the object according to the categories that the subject has *a priori*. According to Nishida knowledge is not the constituting of objects by subjectivity; rather, it is seeing by reflecting both self and all beings inside oneself.

It has been often said by philosophers that one cannot know oneself. Nishida says in his *On the Philosophy of Descartes* (1945) (CVN-11:147–188):

...when you say that you cannot know yourself, you are using the meaning of knowing as recognition of the object. It is reasonable to say so in that sense. You cannot be an object of yourself. But you know you can know yourself. This is why Descartes's first principle says that I think, therefore I am.

All experience occurs inside the self. So, 'place' is required where one sees oneself inside oneself — the place is oneself. Nishida elaborated this idea further in a series of papers published over the next ten years. These are collected in *From the Actor to the Seer* (1927), which reveals a significant shift from existential experience to logic, mediated by the idea of 'place' in Greek philosophy (CVN 4: 3-387). The paper titled 'The Place' is the seventh in this series (CVN 4: 208–289).

'Place of consciousness'

Now what is 'the place' of consciousness? Nishida's place was created by combining all his ideas of self-consciousness with Plato's idea of *chora*⁵ and the fundamental category of judgement mediated by

⁵ Nishida's 'place' was named after the word *chora*, 'space', in Plato's *Timaeus* (2000), but it is not same as Plato's *chora*, or 'receptacle' (CVN 4: 209). For an analysis of the account that Plato gives of the receptacle see Donald Zeyl's "Introduction" to the *Timaeus* (Plato 2000: lxi).

Aristotle's idea of substance.⁶ Aristotle thought that a substance (such as a particular human being) is that which becomes a subject but not a predicate. Judgement becomes possible when a predicate (a universal) encompasses the subject (a particular). In contrast, Nishida considered consciousness as that which becomes a predicate but not a subject. Judgement is possible when the subject is encompassed by consciousness. Here consciousness is the phase of the predicate (called a 'field of consciousness') that contains every being (including the self) inside itself. Thus, he believed that judgement will become possible when the field of consciousness becomes the object of knowledge. Subjectivity becomes embraced by the field of consciousness that includes all beings, including the self.

The model of the place can be imagined as being built up of three-dimensional multiple-layered fields, which together form the sphere of consciousness. The field has a predicate phase on one side, which encompasses all beings in the world including the acting self — referred to as 'thou'. This phase accommodates every phenomenon of conscious action. The other side of the field has a subject phase which is the unity of conscious activity — referred to as the 'I' which can see. Between these two, there is a shadow, corresponding to the absolute will, through which the predicate phase reflects itself. All conscious actions come into existence in this common world of consciousness, which Nishida called a 'field of consciousness'. The subject phase sees the events above on the predicate phase through the shadow. The one to be seen is the one itself. This is like the image in Plato's cave.⁷

⁶ Aristotle's logic of substance can be regarded as the logic of the subject. The substance is not embraced by the predicate; rather, the predicate belongs to the subject. Therefore the substance cannot be recognized by a judgement, but it can only be known by intuition. See for this interpretation Kosaka (2000: 154).

⁷ It would be interesting to compare this model with the model of a person in which subjectivity exists as a point and acts when the self interacts with other beings.

Absolute nothingness

The place should not be regarded as static; in fact, it is infinitely dynamic. The size of the whole place and of each component varies with the interaction and relational changes between the absolute will, the self, other beings, and the subjectivity. The place is a multi-layered structure, and upon reflection it breaks down the floor and moves to deeper and larger layers, towards a bottom. While the field of the consciousness is being expanded gradually, the conscious self will become smaller and smaller. At an ultimate point, the self will vanish and all beings in the field will be seen by the subjectivity only as the shadow of one's self. This is called 'the place of absolute nothingness' where one becomes aware of the true consciousness. This is the place that reflects one's shadow inside oneself. Philosophically, this is said to be 'seeing the mirror that reflects oneself'. The beings seen in this place are considered to correspond to the true, objective knowledge.⁸ The place of the absolute nothingness is the place where not only knowledge, but also feeling and intention come into existence — the place of the origin of everything.

Epilogue

In Nishida's later philosophy, the notion of place was further developed in various directions to accommodate the actuality of the world. His final 'contradictory identity' model was published shortly before his death in 1945 (Hojo 2003: 354–355). Nishida's work has been studied extensively in general philosophy and in the philosophy

⁸ It is interesting that Karl Popper (1972: 106–152), British philosopher of science, had a similar concept of objective knowledge. He says that knowledge in the objective sense is knowledge without a knower; it is knowledge without the knowing subject. "The world 3" of Popper has some similarity to the world of absolute nothingness, although in the former beings exist in an actual world, while in the latter they are still in a conscious one (see also Magee (1985: chapter 5)).

of religion. There are, for example, some interesting papers which draw comparisons between Nishida and such philosophers as Bergson, Hegel, Heidegger, Tanabe and Suzuki. Sometimes, Nishida's idea of place has been discussed in connection with Alfred North Whitehead's 'process philosophy'.⁹ In my opinion, Nishida's works on self-consciousness deserve serious discussion and should be examined within the framework of current philosophy of science, and philosophy of mind, taking at the same time into account the latest scientific achievements.¹⁰

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⁹ For the history and bibliography of the studies of Nishida's philosophy see, e.g., Fujita (1998). Some comparative studies of Nishida and other philosophers may be found in Ueda (1994). Nishida's 'place' in the context of Whitehead's philosophy has been discussed by Yamamoto (1978), Nakamura (1991), Tanaka (1991, 1998), Yamamoto (1994), Hanaoka (1998, 2002) and Nobehara (2001).

¹⁰ Nishida's idea of place has been recently applied in the design of relational life systems. See Shimizu (1999).

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PART II

The Ilya Prigogine Memorial Symposium

Introduction

A Life for the Future

Joseph E. Earley

Four of the papers presented at the Seventh Summer Symposium of the International Society for the Philosophy of Chemistry (ISPC) — held in Estonia in August, 2003 — concerned the work of the Belgian chemist, physicist, and philosopher Viscount Ilya Prigogine (1917–2003), who died in Brussels on May 28, 2003. Those papers are collected in the following pages of this volume.

During his long and highly productive career, Professor Prigogine made major contributions to chemistry, to physics, and to the philosophy of chemistry. Also, to a truly extraordinary extent, he succeeded in bringing the *properly philosophic* importance of chemistry to the attention of the intellectual world. He generously summarized his recent research in a contribution (Prigogine 2003) to the volume that resulted from the Sixth ISPC Summer Symposium that was held in Washington in 2002. This was probably the last publication that he saw through the press.

On the occasion of his receipt of the Nobel Prize for Chemistry in 1977, Professor Prigogine prepared a short autobiography (Prigogine 1977). He introduced that essay by pointing out that, with respect to the relative importance given to the past, the present, and the future, he held an “extreme” view — “I live mostly in the future,” he wrote. He then added: “But the present explains the past.”

The present writer had the great privilege and pleasure of spending much of the Fall Semester of 1976 as a guest researcher in Professor Prigogine’s laboratory in the Université Libre de Bruxelles (ULB).

Joseph E. Earley, Sr.

Since that time Professor Prigogine has been not only an inspiration to me, but also a deeply valued mentor and friend. Professor Prigogine visited me in Washington several times, on his annual trip to the United States to work with his research group in Austin, Texas. In 1981, Professor Prigogine participated in an interdisciplinary conference at Georgetown University marking the hundredth anniversary of the birth of Pierre Teilhard de Chardin, S. J., paleontologist and influential evolutionary thinker.



Figure 1. Ilya Prigogine (right) at Georgetown University in 1981, with Joseph E. Earley, Sr.

On that occasion, Professor Prigogine pointed out that evolutionary philosophy (especially that of Bergson) had exerted a powerful influence on education in French-speaking areas in the early years of the twentieth century, when both Teilhard and Prigogine were

students. In the autobiography, he mentioned the critical importance of philosophical ideas in his own intellectual development.

Since my adolescence, I have read many philosophical texts. I still remember the spell "*L'évolution créatrice*" cast on me. More specifically, I felt that some essential message was embedded, still to be made explicit, in Bergson's remark: "The more deeply we study the nature of time, the better we understand that duration means invention, creation of forms, continuous elaboration of the absolutely new.

A central feature of Professor Prigogine's work, throughout his long and highly productive career, has been exploration of the significance of time — for science and also for other parts of human culture.

The basic laws of classical mechanics — and also those of quantum mechanics — have "time-reversal symmetry". It is not possible for a viewer to tell whether a movie of a collision of two billiard balls (or a film of the interaction of an atom with a quantum of light energy) is being run forwards or backwards. In contrast, time — as we encounter it — is clearly not reversible:

The Moving Finger writes; and, having writ,
Moves on: nor all your Piety nor Wit
Shall lure it back to cancel half a Line,
Nor all your Tears wash out a Word of it. (FitzGerald 1986)

In the nineteenth century, Ludwig Boltzmann famously tried to demonstrate in what way the obvious irreversibility of macroscopic natural processes might arise from underlying microphysical laws that have full time-reversal symmetry. Boltzmann's treatment forms the basis of the majority of contemporary elementary discussions of the reduction of thermodynamics to mechanics — but critics have pointed out fundamental problems in this approach. Bram Edens (2001: 19–21) recently reviewed this question in the course of a general treatment of Professor Prigogine's aims and achievements.

Professor Prigogine's scientific and philosophical efforts — from his work in thermodynamics with his teacher Theophile de Donder (1873–1957), through his famous contributions to understanding self-

organization in far-from-equilibrium chemical systems (made with his large and interdisciplinary research group at the ULB) and on to his recent work (done both at Brussels and in Austin) on nonintegrable microphysical systems (such as on quantum transitions in unstable systems, including decay of excited states of atoms) — have clarified the origin of temporal irreversibility in nature, and explored the philosophical and human significance of that fundamental feature of the world. It can be argued that his most recent studies provide a quite general solution to the problem of how irreversible kinetics arise from reversible dynamics — an alternative to the Boltzmann treatment of that question.

In a contribution that concerns a chemical reaction-type that is of critical importance in the field of self-organization in chemistry, philosopher and historian of science Alexander A. Pechenkin provides an account of the discovery of the Belousov-Zhabotinsky (B-Z) reaction — the paradigmatic example of a self-organizing ‘chemical dissipative structure’. He describes how publication of the initial research dealing with that important process was greatly impeded and delayed — not by interference from agencies of the state, but by opposition arising specifically from within the scientific community. He identifies several sources of this opposition, including an important ‘ideological’ component. Ilya Prigogine’s scientific and philosophical contributions have sometimes also met with hostile reactions from some scientists. Strident attacks (e.g., Bricmont 1996) have been mounted on the basic presuppositions, results, and conclusions of the Brussels-Austin group. As in the case of the initial rejection of the observations on the B-Z reaction, it is not difficult to detect an ideological component in these polemics. As Edens (2001: 27) points out, Prigogine had a more nuanced view of reduction than that entertained by most scientists (especially physicists formed before the last decades of the twentieth century).

Professor Prigogine has been both forceful and explicit in identifying chemistry as that science that deals (exclusively) with systems that do not have time-reversal symmetry. The important differences — that the recent work of the Brussels-Austin school has identified — between such non-integrable systems and the integrable

systems generally studied in theoretical physics is of special significance. Philosopher of science Peeter Müürsepp considers the question of the independence of chemistry with special reference to Prigogine's views on that topic, and to Rein Vihalemm's distinction between 'physics-like' sciences (ϕ -sciences) and sciences with a 'natural history' orientation.

The ubiquity of non-equilibrium self-organization throughout the natural world was a recurring theme of the many articles and books that Professor Prigogine published for a general educated audience. In a striking example of the relevance of self-organization for biology and medicine, neurologist Sławomir Michalak considers certain pathological conditions (varieties of multiple sclerosis) that are characterized by development of concentric patterns on the surface of the human brain. He reviews the prehistory of the concept of spatial auto-organization in German *Naturphilosophie* and in nineteenth century chemical observation of periodic precipitation (Liesegang phenomena), outlines the development of reaction-diffusion models for these processes, involving seminal contributions from Alan Turing and others, and summarizes Ilya Prigogine's contributions to this field. Although present understanding of these important neurological systems is rudimentary, there is real hope that understanding the pathological origins of pattern-formation on the surface of diseased brains may eventually contribute to mitigating afflictions that debilitate many people.

From his youth, Ilya Prigogine had a profound interest in the humanities — literature, art (especially that of India), philosophy, music, anthropology, archeology, sociology, among others. He kept up reading and study in those fields throughout his career, and often organized or inspired conferences that brought leading practitioners of diverse arts and sciences together in fruitful dialog. In contrast, many other prominent physical scientists deal with general humanistic issues quite dogmatically (if at all). Some leading scientists speak on general topics mainly on the basis of prejudices picked up unconsciously in their early years — when they were mainly interested in gaining technical background for future careers in science. It can be argued that taking Professor Prigogine's results seriously both

requires and generates a major shift in fundamental philosophical outlook — a phase-transition in personal metaphysics. (This may partially explain the virulence of some critics.) Philosopher Leo Näpinen's paper on the relationship between man and nature, with special emphasis on Ilya Prigogine's contributions, deals with a field of intellectual activity that Professor Prigogine regarded as of great importance to the long-term flourishing of humankind.

None of the papers in the symposium deal explicitly with an important aspect of Professor Prigogine's career — his major contribution to the construction and fostering of significant institutions. A number of centers all over world devoted to research on non-linear dynamics, complexity, and self-organization owe their origin to his influence and encouragement. His work as Director of the International Solvay Institute for Physics and Chemistry since 1959 has been especially significant. In 1989, Baudouin, King of the Belgians, recognized the importance of his contributions to his adopted homeland by awarding him the rank of Viscount. For many years, Viscount Prigogine was a major force for the flourishing of the support of science in the European Community, and a valued counselor to civic and governmental leaders all over the world. A large part of his success in diverse activities may be attributed to his outstanding personal qualities. In addition to being a scientist of great talent and energy, with a remarkably deep and wide vision, he was also a highly cultured, urbane gentleman — and a person with a deep concern for the long-term benefit of his family, colleagues, and friends.

What might seem to be a trivial story may suggest some of his human warmth and graciousness. When I spent the better part of the Fall semester of 1976 in his Brussels laboratory, I soon learned to stand in awe of many of Professor Prigogine's talents. But the ability that impressed me most was his consummate skill in a daily sweep through the corridors of his large research group to round up a party to fill a lunch table in the ULB cafeteria. This seemed to be an effortless, unpremeditated process guided by pure chance — but yet, when the table was filled, it invariably turned out to be as well organized for fruitful social interaction as if it had been carefully pre-planned by a skillful diplomat. (I never did figure out how he did that.) I consider

myself hugely fortunate to have known Ilya Prigogine, highly honored that I was his friend, and privileged that he was a good friend to me for several decades.

During his lifetime, Professor Prigogine 'lived in the future'. His influence — on science, on general culture, and through his personal qualities on many human lives — will surely persist and grow. His many and varied achievements will continue to live in *our* futures.

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Understanding the History of the Belousov-Zhabotinsky Reaction

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Preliminaries

I. Prigogine writes that “in experimental studies, the Belousov-Zhabotinsky reaction plays the same role as does the Brusselator in theoretical studies” (1980: 121). The Brusselator is a key mathematical model for Prigogine’s non-linear thermodynamics, specifically, a characteristic representation of the phenomena of self-organization. Depending on the circumstances, a wide range of phenomena of self-organization has been observed in the Belousov-Zhabotinsky systems, e.g. the rise of oscillations for a period of the order of a minute and wavelike activity. Hermann Haken also cites the Belousov-Zhabotinsky reaction as a basic model of his synergetics (1977: 9).

The dramatic history of this reaction has been incorporated into scientific folklore and is even outlined in a textbook on non-linear dynamics (Strogatz 1994: 254–255). Several essays on this history have been published. In 1984 historian and journalist V. Poleshchuk published an article on Belousov’s discovery in the famous Soviet literary journal *Novy Mir* (where Solzhenitsyn published his first writings). S. E. Shnol, the academic supervisor of A. M. Zhabotinsky during his university studies, wrote two memoirs concerning Belousov’s discovery of the reaction for which he subsequently became famous, and also about the early stage in Zhabotinsky’s further

development of that work (Shnol 1997, 2001). The prominent biologist A. Winfree published an essay on the Belousov discovery based on his own rich scientific experience and on his conversations with Russian colleagues (Winfree 1987: 661–663). Finally, Zhabotinsky himself wrote a couple of papers on how he elaborated Belousov's discovery, first under the supervision of S. E. Shnol and a bit later independently (Zhabotinsky 1985, 1991). However, no description of this topic from the point of view of a professional historian exists.

The present article focuses on the early events connected with Belousov's discovery. The aforementioned essays report that Belousov's original paper, in which he described the discovery of a homogeneous oscillatory reaction and proposed a tentative mechanism for that process, was rejected by two main Soviet chemical journals *Zhurnal obshchey khimii* (The journal of general chemistry) and *Kinetika i kataliz* (Kinetics and catalysis), in 1951 and in 1955, respectively. Belousov finally managed to publish a brief abstract in the obscure proceedings issued by the Institute where he was employed as head of a laboratory (Institute of Biophysics at the Ministry of Public Health). Belousov died in 1970. His full paper was published only posthumously in 1981. An English translation of the 1951 version of his paper appeared in 1985 (Field and Burger).

Interestingly, "external" forces cannot be blamed for this rejection. Neither the Communist Party nor the state ideologists intervened. It was the scientific community itself, as represented by the editors of scientific journals and their referees, that refused to accept Belousov's discovery.

In order to explain the 1951–1955 situation, Arthur Winfree points to "the resistance of human nature to observations that do not fit into existing theory" (Winfree 1987: 661). S. E. Shnol displays a similar attitude.

The main obstacle proceeded from textbooks on equilibrium thermodynamics. A well-educated person could not imagine a macroscopic order in the chaotic motion of a tremendous amount of molecules. He could not believe that the mole-

cules could altogether come to the one state and then to the other state. (Shnol 1997: 151–152)

However, he places emphasis on the moral aspect of the situation as well: influential Soviet chemists did not want to concern themselves with facts that were provided by an experimentalist engaged in applied research. Poleshchuk also emphasized the moral aspect. He referred to Belousov's inscription on a book given by him as a gift to his life-long friend: "Don't be ashamed of not knowing, be ashamed of not willing to know." (Poleshchuk 1984: 201) Although this inscription was not directly connected with Belousov's unsuccessful struggle for publishing his results, Poleshchuk used it to evaluate the editor's attitude to Belousov's paper.

I am going to treat the subject in terms of the philosophy of science. However, first I will call attention to some historical details. The situation with Belousov's discovery was more complicated than the articles mentioned above might suggest. In 1949, i.e. two years before Belousov's first attempt to publish his results, *Zhurnal Fizicheskoy Khimii* (Journal of Physical Chemistry) published an article concerning oscillatory homogeneous reactions. It was I. E. Salnikov's article that summed up a series of his studies conducted together with David A. Frank-Kamenetsky at the Institute of Chemical Physics since 1941. Frank-Kamenetsky had begun the study of chemical oscillations at the end of the 1930s. In 1940 he published an article on the oscillations of cool flames — he was the first to obtain these oscillations for a closed system. In 1947 Frank-Kamenetsky published a textbook which ran into three editions. The title of that text was *Diffusion and heat transfer in chemical kinetics*. The book contains a chapter "Periodic processes in chemical kinetics".

It should also be mentioned that in 1957 Shnol started to publish his results concerning the oscillations of ATP-ase activity of actomyosin (a kind of protein). Shnol told me that he experienced difficulties as he attempted to publish his results in the leading journals of the Academy of Sciences. Nevertheless, his articles had been published and, as noted above, Shnol suggested to his student Zhabotinsky that he might continue Belousov's research as his own

dissertation problem. This was at the Physics Faculty of the Lomonosov Moscow State University in 1961. It is well known that, at that time, dissertation topics had to be approved by the Chair and by the Scientific Council of the faculty (department). This means that, at the beginning of the 1960s, Belousov's discovery was approved by those faculties. Zhabotinsky successfully conducted his research which soon became independent and resulted in a series of publications in the most prestigious Soviet scientific journals, and for which he, finally, was awarded the Lenin Prize (the highest Soviet scientific honor) in 1981. Belousov's name was added to the list of nominees through Shnol's efforts .

At the end of the 1950s, D. S. Chernavsky who worked at the Physics Institute of the Academy of Sciences, published a number of articles on periodic processes in photosynthesis. So, at the beginning of the 60s, one can observe a "scientific movement" towards the legitimization of chemical oscillations. Articles about chemical oscillations appeared in print a bit earlier than Belousov's unsuccessful attempt to publish his results, and they also appeared a bit later. Why then was Belousov's paper rejected? And, conversely, why did Belousov's contemporaries succeed in publishing their results on chemical oscillations?

In the following section I shall outline the methodology of my article. This is centered around two concepts: "paradigm" and "ideology". The third section treats the ideological context in which Zhabotinsky began his research under the supervision of Shnol. The fourth section deals with Zhabotinsky's work in the context of non-linear dynamics (the theory of non-linear oscillations). The fifth section shows that Zhabotinsky and his collaborators came close to the paradigm of synergetics.

The methodology: paradigm and ideology

In my recent article (Pechenkin 2002) I distinguish between two intellectual constraints on research — paradigm and ideology.

Following Thomas Kuhn I hold that a paradigm encompasses problem-solving activity, since it involves typical conceptual tools, models, and shared examples; it reduces problems to "puzzles". To describe a paradigm one must mention its: 1) symbolic generalizations, 2) ontological model, 3) values, and 4) shared examples. In the spirit of Quine, I shall mean by "ideology" the language resources of a theory — the particular descriptive terminology which the theory brings to science. The ideology can also be recognized as a set of concepts which can be expressed in the language of the theory. While the paradigm involves problem-solving activity, the ideology provides a preliminary interpretation of facts and indicates what is scientifically important. While the paradigm guides the formation of a theory, the ideology allows for the expansion of the theory into associated areas where it points to new interesting phenomena and poses new problems.

By referring to "examples", "heuristic models", and "values" as the components of a paradigm, Kuhn partially expressed in this concept what I call ideology. Kuhn sometimes tended to distinguish between the paradigm as ideology and the paradigm as a set of "rules for research". For him, "normal science" was initially formed within the framework of crude analogies, models, or in a word, within the framework of what is called ideology here. By means of crude analogies, models, etc. empirical facts were interpreted as interesting and problems were identified. When Kuhn was writing about crises and anomalies, he turned to the paradigm as a set of rules. Crises and anomalies appeared in the course of the problem-solving activity which the rules encompassed.

In contrast to Kuhn, I regard ideology as an intellectual machinery in its own right. The ideology is an essential part of a paradigm, but *it can go beyond the paradigm and prepare the rise of a new paradigm*. A scientific community, if it is authoritative, can extend its shared concepts and examples far beyond the area in which its rules and methods are effective, i.e. beyond the sphere of its problem-solving activity. In other words, an authoritative scientific community has authoritative concepts and examples. Ideology comprises a legitimating framework which indicates what is worthy of attention,

allows the posing of problems, and hence provides a prior interpretation of phenomena. However, ideology is unable to reduce problems to puzzles. It only prepares the ground for problem-solving activity, which is provided by the extension of the old paradigm or by the formation of a new paradigm.

In the present paper (and in my article published in *Studies in History and Philosophy of Modern Physics*) I argue that the history of Belousov's discovery cannot be understood solely within the framework of Kuhnian paradigms. These paradigms should be supplemented by ideologies (understood in the sense of Quine).

True, Kuhnian paradigms shed light on the rejection of Belousov's paper from 1951–1955. As mentioned above, Winfree emphasizes that the Belousov discovery did not fit into the framework of contemporary chemical theories, while Shnol points out that it was incompatible with chemical thermodynamics. Winfree's and Shnol's interpretations should each be elaborated more carefully. Belousov's discovery did not contradict thermodynamics or any other existing scientific theory. Moreover, in his 1974 book Zhabotinsky explained the situation with Belousov's discovery by pointing to a confusing identification of the stationary state of a chemical system with its equilibrium state (Zhabotinsky 1974: 43). However, this explanation does not concern the historical reasons: the chemists who refused to accept Belousov's discovery, could not read Prigogine's books on non-linear thermodynamics and Zhabotinsky's own papers. I believe that the situation can be elucidated with the help of Kuhnian paradigms. Belousov's discovery did not fit into the paradigm of classical chemical thermodynamics. This paradigm can be described as follows: 1) ("symbolic generalizations") thermodynamical functions characterize how a system is approaching its equilibrium state; 2) ("ontological model") every free system spontaneously arrives at dynamic chemical equilibrium; 3) ("values") thermodynamics provides the basis for the study of chemical processes; and 4) ("shared examples") simple physical processes, say, equilibrium between a liquid and its vapor, the irreversible process of mixing of two gases.

Belousov's reaction, in turn, presupposes the following: 1) Although thermodynamic functions are monotonic, the state of some

systems is described by periodic functions; 2) The evolution of the system results in a stable stationary structure constituted by ordered transformations of molecules, whereas thermodynamic equilibrium, at which every system should spontaneously arrive, is provided by a chaotic set of molecular processes (approximately half of particles participate in the forward reaction, while the other half participate in the reverse reaction, and as a result there are no net changes in the system); 3) The Belousov discovery throws doubt on standard thermodynamics; 4) "Shared thermodynamic examples" turn out to be irrelevant.

It should be stressed that Belousov discovered a homogeneous chemical reaction that was periodic. Establishing the homogeneity of his system was his challenge. Heterogeneous periodic reactions had been known since the end of the nineteenth century (the most famous example was the "Liesegang rings", discovered by R. Liesegang, a specialist in photograph chemistry, in 1896), and they were accepted by chemists. In 1898, Wilhelm Ostwald put forward a theory of the Liesegang rings, and other theories followed. If anybody, say, Frank-Kamenetsky described an oscillatory reaction, chemists treated it as belonging to the class of heterogeneous reactions. By contrast, Zhabotinsky recalled that, even in the mid-1960s, he had to prove that the Belousov reaction was actually homogeneous (Zhabotinsky 1985: 2).

In his Foreword to the Russian edition of (Field & Burger 1985) Zhabotinsky regarded this difference in the chemists' attitudes toward homogeneous and heterogeneous reactions as an enigma. Zhabotinsky wrote that the only explanation was psychological: people are accustomed to come across periodic mechanical and physical processes, and heterogeneous reactions presupposed mechanical and physical processes in their structure. I think that this explanation can be improved by invoking the above-mentioned paradigm of classical chemical thermodynamics. It turned out that this paradigm reduced heterogeneous oscillatory reactions to "puzzles" while relegating homogeneous oscillatory reactions to the disreputable category of anomalies. Let us return to the "Liesegang rings" (see also Michalak's paper in the present volume). Liesegang placed a gelatin solution

containing potassium bichromate (bichrome) on a glass plate. Once the gelatin had set, he dropped silver nitrate in the center of the plate. It was known that the interaction of bichrome and silver nitrate precipitated silver bichromate, which was purely soluble. However, Liesegang observed that instead of a continuous spot of the deposit he had "rings" which looked like the annual rings from the cross-section of a tree. The precipitation proceeds by means of waves.

In his explanation of the "Liesegang rings" Wilhelm Ostwald used the concept of a metastable state — i.e. the quasi-equilibrium state which had (in contrast to the true equilibrium state) low stability. Ostwald suggested that nitrate and bichromate move to meet each other, so that a superconcentrated solution of silver bichromate is formed. From the thermodynamic point of view this solution is in a metastable state. It goes into its ordinary equilibrium state when an act of precipitation takes place. After the precipitation the process of the substance transfer again intensified and a subsequent portion of superconcentrated solution arose.

So, the "Liesegang rings" were incorporated into the paradigm of chemical thermodynamics. To understand the way in which Belousov's reaction was adopted by the chemical community, we need to shift our attention to the other intellectual constraint, which I discuss in the present article, namely, to scientific ideology. It is the ideology of the expansion of biology into chemistry that formed the context wherein Zhabotinsky started his research under Shnol. More specifically, this research was legitimated by the ideology of biorhythms (and biological clocks).

The ideology of biorhythms and biological clocks

The expansion of chemistry into biology is well-known. The rise of biochemistry and molecular biology manifested the expansion. However, by the end of the 1950s the opposite tendency had also emerged. This was the tendency to apply some fundamental biological categories in chemistry: first of all, the categories of evolution and

individuality. This was accompanied by institutional innovations. In 1958 the Chair of Biophysics was established at the Physics Faculty of the Lomonosov Moscow State University. The Chair of Molecular Biophysics was organized at the Faculty of Molecular and Chemical Physics of the Moscow Institute of Physics and Technology in 1959. (Later this Chair gave life to a new faculty of this institution, the Faculty of Physical and Chemical Biology). Shnol gave a lecture course in biochemistry at the Chair of Biophysics, Zhabotinsky was a graduate student at that Chair. It should also be noted that Zhabotinsky's first paper appeared in the journal named *Biophysics*, and that in this paper he stressed the biological importance of Belousov's reaction.

To illustrate the ideological penetration of biology into chemistry let me cite the Nobel Laureate, chemist N. N. Semenov, who headed the Institute of Chemical Physics where Frank-Kamenetsky was employed. Acting as the main chemical ideologist in the USSR, he repeatedly called for the adoption of the "experience of life science in chemistry". In particular, Semenov said in his 1970 address (Semenov 1981: 192–193):

In the process of its evolution the nature created molecular machines of the highest degree of exactness and of rapidness of action, machines of extraordinary perfection... By using the principles of chemistry of living organisms it is possible to construct a new chemistry, that is, a new control of chemical processes. This chemistry will use the principles of synthesis of the large protein molecules, catalysts of the highest specificity will be created according to the principles of ferments ...

It is not difficult to notice that this ideology can be traced back to the "natural automata" in Leibniz's and Kant's writings.

But here it should be noted that the ideology which directly shaped the early context of Zhabotinsky's research was the ideology of biorhythms and biological clocks. Studies in biorhythms, i.e. in daily periodic physiological changes of organisms, can be traced back to the nineteenth century. In the 1930s biologists launched research into the

genetic aspects of endogenous biorhythm, i.e. biorhythms that are autonomous with respect to astronomical cycles. These studies were presumably experimental. But they involved a speculative element. Searching for the foundations of biological rhythms biologists tended to discuss the organization of living things and to presuppose an hierarchy of periodic processes in them.

One of the "classics" of the biorhythm studies was H. Bünning, who began to study periodicity in the behavior of plants in the 1930s. In 1958 he summed up his research in the book *Die physiologische Uhr* (Berlin: Springer) which gained popularity in the Soviet Union (at least Chernavsky, Shnol, Zhabotinsky and others referred to Bünning's book). In 1961 an extensive Proceedings of an international conference dedicated to biorhythms and biological clocks was issued. This book was translated into Russian with Shnol acting as editor. Shnol wrote in his Foreword (Shnol 1964: 7):

The crux of the problem is to prove that the majority of living organisms have an internal ability to measure time that is transmitted by heredity. In normal conditions the work of endogenous "biological clocks" is correlated with periodic processes in the environment.

Shnol added in a speculative manner:

What is the nature of the processes which result in daily periodicity?... It is possible that they are based on a combination of diffusion and the processes of biosynthesis, the combination which results in periodic changes of the properties of cells. Now it is difficult to say to what extent diffusion and processes of biosynthesis can result in periodic processes with periods of short duration (a few minutes or less). Anyway it is clear that the problem of the mechanism of chemical and physico-chemical periodic processes has gained important significance...

It is probable that daily periodicity is based on chemical or physico-chemical processes. Their duration is small and within a daily cycle a multitude of "elementary chemical oscillations" takes place. Here the analogy between biolo-

gical clocks and ordinary clocks comes to mind. The accuracy of mechanical clocks is determined by the stability of frequent pendulum oscillations.

As was mentioned above, in 1957 Shnol published an article concerning the oscillations of ATP-ase activity of actomyosin. This article was highly empirical: the author insisted that empirical facts themselves showed periodicity. As he told me, a bit later he wrote another article which was never published, and where he allowed himself to be somewhat more speculative. Nevertheless, the idea of fundamental chemical (or physico-chemical) periodic processes in organisms was in the air during the late 1950s. As Shnol writes in his book (1997: 156–160) he learned by chance about the content of Belousov's discovery (not about Belousov). He began to search for the person who had discovered chemical oscillations, and in 1958 he finally met Belousov. Belousov showed Shnol his 1951–1955 manuscript, but he refused to cooperate in research. Shnol, however, convinced Belousov to publish an abstract of his paper.

Zhabotinsky started his work in the context of biological rhythms and clocks. But this ideology played no significant role in his work, although it allowed Shnol to legitimate this work. Zhabotinsky formulated his problems and results by using the language of the physico-mathematical theory of oscillations. This ideology — the ideology of self-oscillations — will be described in the next section. Here let me note that material of the 1966 First All-Union (National) Conference on Oscillatory Processes in Chemistry and Biology shows that two ideologies were present at that conference. (The conference was held in Pushchino-na-Oke, a small city of Moscow region, where the Institute of Biophysics of the Academy of Sciences was established in 1963). A series of articles by D. S. Chernavsky on biological periodic processes was mentioned in section 1. In this series also, two ideologies are apparent. One reads in D. S. Chernavsky's and M. Chernavskaya's article that "by nature every internal rhythm is nothing more and nothing less than a self-oscillatory regime of internal chemical reactions" (1960: 632).

The ideology of self-oscillations

In my previous article (Pechenkin 2002) I describe the rise and development of the ideology brought to science by the physico-mathematical theory of non-linear oscillations — the ideology of self-oscillations. Here I reproduce the main points of my argument in order to describe the extension of this ideology to chemistry. The ideology of self-oscillations was the ideology of a powerful scientific community which is usually called “the Mandelstam school” (or “the Mandelstam-Andronov school”). “Self-oscillations” is a central concept of the theory of non-linear oscillations which was developed by this community — it was the characteristic message of the theory. In its early stage, the theory of non-linear oscillations was simply the theory of self-oscillations. This concept enabled broader application of the theory of non-linear oscillations whose original domain was lumped systems — i.e. application to continuous media and the subsequent progress toward synergetics. By combining the Greek word “avto” (“auto”) and the Russian word “kolebaniya” (“oscillations”), Mandelstam’s graduate student A. Andronov invented a very expressive word that covered not only his physico-mathematical ideas, but also his visualizations and examples (first of all, these were the simple tube generator, the Froud pendulum, and the clock). In the course of its ideological application, the concept of self-oscillations was greatly extended, it became vague and diffuse, and related concepts such as self-waves and self-structures appeared.

In brief the story runs as follows. In 1925 Leonid I. Mandelstam, who graduated from Strasbourg University in 1902 and started as a radiophysicist and optician at the Strasbourg Institute of Physics, overtook the Chair of Theoretical Physics at the Moscow State University. Around him a group of talented scientists was formed. In 1927 Mandelstam set his graduate student A. Andronov the problem of improving the mathematical technique with the help of which a radio-engineering device (the tube generator) was approximately described. Andronov’s work resulted in important conceptual innovations. In his 1928 paper and in his subsequent Ph.D thesis, a rigorous mathematical theory of the oscillations typical for a tube

generator and evident in many customary devices (say, a clock) and in living beings (say, beats of the heart) was presented. Andronov turned to the qualitative theory of differential equations developed by Henri Poincaré in another context. This theory yields strict (although qualitative) solutions of nonlinear differential equations. It provides the methods of what Andronov and his coworkers called "qualitative integrating". This means methods for determining the states of equilibrium implied by the differential equation, for analyzing their stability, for recognizing the periodic solutions represented by closed curves, for finding out whether they are stable, etc.

Andronov demonstrated the connection between Poincaré's limit cycles and the aforementioned oscillatory phenomena (in tube generators, clocks, etc). He put the general problem of integrating the differential equation:

$$d^2x/dt^2 + \gamma dx/dt + \omega^2 x = f(x, dx/dt),$$

where x is the generalized coordinate (e.g. the current, excursion of a pendulum), t is the time, γ is a damping factor, ω is the eigenfrequency (i.e. the frequency of oscillations which would take place if the damping and the energy source had been eliminated), $f(x, dx/dt)$ is a nonlinear function describing how to operate the energy source included into the control system of self-oscillatory design. The limit cycle is a closed trajectory (hence, the trajectory of a periodic solution) such that no trajectory sufficiently near to it is also closed. In other words, a limit cycle is an isolated closed trajectory to which all neighboring trajectories converge in the course of time (at $t \rightarrow \infty$ or $t \rightarrow -\infty$). This means that every trajectory whose starting-point is sufficiently near to this cycle either winds itself upon it or unwinds from it. In the former case we have a stable limit cycle, in the latter case we have an unstable limit cycle.

After a number of successful studies (which Andronov partially conducted with A. Vitt, another former student of Mandelstam) the concept of self-oscillations gained popularity. It turned out to be the conceptual center of the book *The theory of oscillations* (1937) by Andronov, Vitt and Khaikin which appeared in three Russian editions

and was twice translated into English (1949, 1965). (The book was written by Andronov in cooperation with two other former graduate students of Mandelstam, Vitt and Khaikin. As Vitt was arrested, his name never appeared in the first edition). In connection with the concept of self-oscillation the book also represents other major conceptual innovations of the Mandelstam-Andronov school, namely, the concepts of bifurcation and roughness (structural stability). After World War II two books dedicated to the elaboration and popularization of the concept of self-oscillations were published (Teodorchik 1944, Kharkevich 1953). K. Teodorchik's book ran into three editions. "The phenomenon of self-oscillations occurs in nature at every step," G. Gorelik, Mandelstam's former student, wrote in his popular text-book *Oscillations and Waves* (1950).

At the beginning of the 1930s Andronov moved to Gorky city (now: Nizhny Novgorod) where a scientific community was formed around him. This community can be considered as a branch of the Mandelstam school. The main concern of Andronov's group was to develop the concept of self-oscillations for multidimensional systems so that it would be applicable to control engineering and to continuous media. Y. I. Neymark, Andronov's former graduate student, told me in a conversation:

I was like a bloodhound on the scent of self-oscillations. Where did I not see self-oscillations? My graduate student Y.I. Gorodetsky was concerned with self-oscillations in metalworking... I dealt with self-oscillations in burning, now I am concerned with — you have seen the journal *Priroda* — self-oscillations in society. [Here, Neymark is referring to his article (1991) in the popular scientific journal "Priroda". — A.P.]

Let us return to chemical oscillations. In section 1 I mentioned I. Salnikov who published an article on homogeneous oscillatory reactions in 1949. Salnikov was a student of G. Gorelik whose text-book has just been mentioned. His research into chemical oscillations was initiated by Andronov. In his first article on self-oscillations Andronov pointed to periodic reactions as an example of self-

oscillations (Andronov 1929: 561). He referred to R. K. Kremann's *Die periodischen Erscheinungen in der Chemie* (Stuttgart: Enke, 1913). This reference was purely ideological: Kremann's book does not mention any self-oscillatory chemical reactions, if by "self-oscillations" we mean phenomena described by the above type of differential equations whose "qualitative integration" yields limit cycles.

Andronov also referred to A. Lotka's writings (Andronov 1929: 561, Andronov and Khaikin 1937). Lotka's 1910–1920 articles are very important in our context. However, Lotka had not arrived at the self-oscillatory model of chemical reactions. In his 1910 article Lotka proposed equations for dissipative systems, i.e. equations describing damping oscillations. He considered the following mechanism:



(where $\xrightarrow{\leftarrow}$ designates self-catalysis (or auto-catalysis), that is, $X+Y \rightarrow 2Y$),

which corresponds to the following system of equations:

$$dx/dt = k_0A - k_1xy$$

$$dy/dt = k_1xy - k_2y.$$

In 1920 in an article published in *The Journal of American Chemical Society* Lotka improved his mathematical model. He considered the following chemical reaction:



And he formulated the following equations:

$$dx/dt = k_0Ax - k_2xy$$

$$dy/dt = k_2xy - k_3y.$$

These equations already describe undamped oscillations. But these oscillations are not self-oscillations because they are unstable. By referring to Lotka's model as a self-oscillatory model Andronov

suggested that if this model was modified, it would give self-oscillations.

When setting Salnikov the task of studying chemical self-oscillations, Andronov suggested that Salnikov should continue Lotka's work and that he should put his work on experimental basis. Salnikov was sent to cooperate with Frank-Kamenetsky at the Institute of Chemical Physics. As was noted, Frank-Kamenetsky had already described the oscillatory behavior of cool flames. As Salnikov wrote in his recollections, it was his aim to turn Frank-Kamenetsky into an adherent of self-oscillations (Salnikov 1992: 8). And indeed, Frank-Kamenetsky referred to self-oscillations in his 1942 article. But this reference was merely ideological: Frank-Kamenetsky did not really apply Andronov's methods; instead, using Andronov's terminology, he only interpreted what he had obtained by his own methods. Frank-Kamenetsky proceeded from Lotka's 1920 model and additionally assumed the existence of "active by-products" whose concentrations increase according to the law

$$x = x_0 \exp(k_1 a t),$$

where t is time, a is the concentration of the co-reagent, k_1 is the constant of the rate (and correspondingly for y). By using the Lotka equations he calculated the critical values of x and y (x_{cr} is the value of x at which dy/dt turns out to be zero, and likewise for y). He showed that on these assumptions the concentrations x and y oscillate around x_{cr} and y_{cr} .

In 1943 Frank-Kamenetsky and Salnikov published an article in *The Journal of Physical Chemistry*. They tried to solve the problem within the framework of the Andronov paradigm (not only using his ideology). By developing the Lotka equations they tried to obtain equations which would describe the self-oscillations of cool flames. As Salnikov pointed out later, their attempt was not quite successful. Lotka's equations are unsuitable for processes which are not isothermal (Salnikov 1992: 10).

In 1949 Salnikov published an article to which I have referred above. He used the idea of thermal catalysis at which he had arrived

with Frank-Kamenetsky. The idea is the following: the Arrhenius equation

$$k = A \exp(-E_{akt}/RT),$$

where k is the constant of action, E_{akt} is the energy of activation, T is temperature, shows that if a reaction is heat-producing, then we have an increase in temperature, and hence an increase in the velocity of the reaction. Salnikov formulated a system of equations containing exponents and yielding a limit cycle under some conditions (Salnikov 1949).

In the context of my present paper, however, the ideological contribution of Frank-Kamenetsky and Salnikov is of more importance. Their work played some role in turning Zhabotinsky to the ideology of self-oscillations. As was mentioned, Zhabotinsky started his research in the framework of the biorhythm ideology — the ideology which guided his teacher Shnol in his studies of oscillatory biochemical reactions. Zhabotinsky read Frank-Kamenetsky's and Salnikov's writings charged with the ideology of self-oscillations. He also read Chernavsky's writings where the ideology of biorhythms was used alongside with the ideology of self-oscillations. As noted in the previous section, an important conference on oscillations in chemistry and biology was held in Pushchino-na-Oke in 1966. Frank-Kamenetsky said in his address to this conference: "We must give a proper language to our science [he meant the study of chemical oscillations — A.P.]; the best way is to use the language of radio-engineering because this is the most advanced field in the study of oscillations." (Frank 1967: 40)

In 1965 Zhabotinsky published (with his coauthor Korzukhin) an article "Mathematical modeling of chemical and ecological self-oscillatory systems". However, as recalled by Shnol, he was inclined to use the conceptual tools of the qualitative theory of differential equations from the very beginning of his research. Zhabotinsky's major book *Concentration self-oscillations* which summarized his research was published in 1974. In the Foreword he wrote that he belonged to the fourth generation of the Mandelstam school. He regarded his father Mark Zhabotinsky as his main teacher. Mark Zhabotinsky had been a student of Strelkov who in turn was

Mandelstam's student. In this Foreword Shnol was only included in the general list of persons who influenced Zhabotinsky.

When I spoke with Shnol I felt that something was wrong in his relations with Zhabotinsky. "Zhabotinsky is a person whose self-estimation is too-high," Shnol said. I think that a historian must be very careful when describing the teacher-student relations. But the following can be definitely said: there is an ideological divide between Shnol and Zhabotinsky. By comparing Zhabotinsky's *Concentration self-oscillations* and Shnol's *The physical and chemical factors of biological evolution* (1977) one can notice that the former is imbued with the physical ideology of self-oscillations, while the latter retains the ideology of biorhythms and biological clocks (in his book, Shnol connected this ideology with M. Eigen's idea of hypercycles).

Zhabotinsky's work consisted of two parts: 1) he elaborated the mechanism and, eventually, the mathematical model of Belousov's reaction; 2) he proved that a homogeneous chemical oscillator is possible. The first part was quite paradigmatic: Zhabotinsky worked within the framework of Andronov's paradigm and his puzzle was how to find a limit cycle corresponding to the Belousov oscillator. The second part of the problem was solved by "turning around" the Bodenstein method of quasi-stationary concentration. This problem cannot be regarded as a puzzle within the paradigm of non-linear oscillations. Moreover, Zhabotinsky and his co-author here came close to another paradigm — the paradigm of synergetics (see next section). But the ideology of self-oscillations was also in operation when Zhabotinsky proved that homogeneous chemical oscillators are possible. The thing is that Zhabotinsky proved that self-oscillatory homogeneous reactions are possible.

Let us turn to the first part of Zhabotinsky's research. The research was carried through along two lines: 1) the improvement of the Lotka model in such a way that this mathematical model would represent self-oscillations; 2) the improvement of Belousov's mechanism of his reaction in such a way that this mechanism would be self-oscillatory. These two lines had converged in the late 1960s: in 1971 the self-oscillatory model of the Belousov reaction (or more exactly, of the Belousov type of reaction) was published (Zhabotinsky et al. 1971).

Toward the paradigm of synergetics

The second part of Zhabotinsky's research (ideological with respect to the theory of non-linear oscillations) consists in the following. Zhabotinsky and his coauthor M. Korzukhin showed the possibility of a self-oscillatory mechanism which obeyed the law of reactant masses — the basic law of chemical kinetics. To put it differently, they showed that self-oscillations are possible in a homogeneous chemical system.

The idea was to "turn around" the Bodenstein method of quasi-stationary concentrations. This method allowed one to simplify the kinetics of a reaction by separating "fast" and "slow" variations of concentrations and then by neglecting some of the variations. The mathematical scheme of the method runs as follows:

Let the mechanism of a reaction be represented by the system of differential equations

$$\begin{aligned} dx_i/dt &= f_i(x,y) \\ \varepsilon dy_j/dt &= g_j(x,y). \end{aligned}$$

The first set of equations represents "slow motions", the second set represents "fast motions". If $\varepsilon \rightarrow 0$ and certain mathematical conditions are fulfilled, this system converges to a system which is simpler because its order is less, namely, it converges to

$$\begin{aligned} dx_i/dt &= f_i(x,y) \\ 0 &= g_j(x,y). \end{aligned}$$

To turn this method around means the following: 1) to construct a simple, idealized model of the chemical reaction — the model which may be "nonchemical", i.e. this model may contain equations that do not obey the law of reactant mass; 2) to modify this model — to make it more complicated by adding new variables (in particular, to introduce the separation of "slow motions" and "fast motions" into the model), and to arrive at a "chemical" model consistent with the laws of chemical kinetics. This more complicated model must asymptotically converge to the former model.

Zhabotinsky and Korzukhin proved that a “nonchemical” oscillatory kinetic model can be so modified that it results in a “chemical” oscillatory model which asymptotically converges to the “non-chemical” one.

Let me bring a simple example to illustrate this operation (Zhabotinsky and Korzukhin 1967: 225). The example concerns a reaction whose idealized simple description is “nonchemical”. This description is a simple differential equation:

$$dx_1/dt = -x_2 .$$

The reaction is represented as a reaction of decomposition of the order zero. The “nonchemical” character of the description follows from the fact that it eventually leads to negative values of the concentration x_1 . By adding “fast motions” we transform its description into a system of equations consistent with chemical kinetics:

$$dn_1/dt = -(1/\epsilon) n_1 n_0$$

$$dn_0/dt = -(1/\epsilon) n_1 n_0 + n_2$$

Of course, this example does not show that the self-oscillatory mathematical model is consistent with the law of reactant masses. The above equations are not oscillatory at all. The example only proves that a very simple mathematical model with “non-chemical” x_1 and x_2 can be transformed into a model consistent with the law of reactant masses. The latter model asymptotically converges to the original equation.

By introducing the Bodenstein method into the context of the theory of differential equations, Zhabotinsky and Korzukhin came close to Haken’s synergetics and to Prigogine’s non-linear thermodynamics. Both of these latter approaches use the “steady state condition” which can be understood as a generalization of the Bodenstein condition of a quasi-stationary state (Haken 1977: 9, Nicolis and Prigogine 1989: 3,6). It should be emphasized that this condition has a paradigmatic significance for Haken and Prigogine. Haken, for example, used essentially the same condition in his theory of the laser. Let us take a simple one-mode laser. After certain reasonable approximations, the theory leads to the following systems of equations:

$$dn/dt = GnN - kn$$

$$dN/dt = -GnN - fN + p,$$

where n is the number of photons, N is the number of excited atoms, G is the gain coefficient for stimulated emission, k is the decay rate due to the loss of photons by mirror transmission and scattering, f is the decay rate for spontaneous emission, and p is the pump strength. Suppose that N relaxes much more rapidly than n . Then we may use the quasi-stationary approximation and take that dN/dt equals zero. By expressing N in terms of n we arrive at a first-order system for n . In Haken's words, the behavior of N is slaved to that of n which is an order parameter.

In his *Synergetics* Haken treats chemical reactions, where spatio-temporal oscillations occur, with the help of the steady state conditions. He writes that "the onset of the occurrence of such structures is governed by principles analogous to those governing disorder-order transitions in lasers, hydrodynamics, and other systems" (Haken 1977: 9).

As Haken himself pointed out, his order parameters were analogous to the order parameters in L. D. Landau's theory of second-order phase transitions (1977: 180). However, there is another source of Haken's synergetics in the Soviet science. This is the separation of "slow" and "fast" motions in the writings of the Mandelstam-Andronov school. Originally this operation had an auxiliary function: since Andronov's and Vitt's paper (in 1930) on the relaxation self-oscillations it helped to treat "puzzles". But gradually it became more important. The theorems of A. N. Tikhonov on differential equations with small parameters (1948, 1952) provided the necessary background for the separation. In particular, this operation culminated in Zhabotinsky's and Korzukhin's work. Zhabotinsky and Korzukhin used it in the paradigmatic part of their work: it allowed them to develop the Lotka equations for auto-catalysis and to obtain a limit cycle. Apart from this, they solved a more general problem: they theoretically showed that the concentration self-oscillations are consistent with chemical kinetics.

Conclusion

Belousov failed to publish his celebrated paper because there was no scientific ideology underlying this paper, i.e. he did not belong to a powerful scientific community. His discovery was first accepted within the ideological framework of biorhythms and biological clocks. Zhabotinsky's research, however, was guided by the ideology of self-oscillations, and afterwards by the paradigm of self-oscillations. The ideology of self-oscillations not only prepared the introduction of the corresponding paradigm, but it also led to a new paradigm — the paradigm of synergetics. Thus, sometimes ideological descriptions in theoretical language turn out to be every bit as important as theoretical explanations and predictions.

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Chemistry as an Independent Science

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Introduction

It seems that we, philosophers of science, all know what we are talking about when we speak about chemistry. Normally, everybody agrees that chemistry is a branch of science quite close to physics. But if it is quite close to physics, why cannot it be included in physics? And what are the links between chemistry and biology? These are some of the central concerns of my paper.

We might also put the main issue as follows. Science needs to explain reality. Normally, different branches of science explain somewhat different sections of reality — to some extent at least, although there are large overlapping areas. Our problem is whether there is something unique in reality which cannot be explained by physics or biology, for instance, and which only chemistry can explain? According to Jürgen Mittelstrass we may ask: “If nature does not distinguish between physics, chemistry, and biology, why should those sciences that investigate nature do so in an unshakeably disciplinary manner?” (Mittelstrass 2002: 49)

The problem we are facing is connected to the issue of the unity of science as well. It may be that we are witnessing the formation of a new solid foundation for unified science just on the basis of chemistry.

Chemistry and Physics

There are two common ways of comparing chemistry and physics to each other. The problem of their relationship is often regarded as that of the reducibility of chemical theories and entities to physical theories and entities. But it is trivial that different fields of knowledge, pertaining to different fields of reality, differ due to their different content (Vihalemm 2001: 186). Therefore, it seems more reasonable to turn to the possible methodological identification of chemistry with physics. If we try to compare chemistry with physics (or any other branch of science), we have to find the appropriate methodological basis for fulfilling this task.

Chemistry certainly is a natural science. It falls into the same category with biology, physics and other branches of natural science. Until quite recently, no one seriously thought about asking whether chemistry could also be regarded as a historical science. Here, by “historical” we don’t mean “having a history”. History in this sense is necessarily there. We mean “historical” in the sense of being dependent in its results on the direction of time. Again, one might say that some such dependence is obvious. Empirical research cannot be done instantaneously — it occurs in time. And it is specific to chemistry that it produces some of the stuff it deals with.

We can put the problem a bit differently: is chemistry a constructive-hypothetico-deductive discipline (a ϕ -science) or a classifying-descriptive-historical discipline (a non- ϕ -science)? Here it seems reasonable to agree with Rein Vihalemm (2001: 186) who holds that chemistry should aim at the co-operation of these two approaches. The late Ilya Prigogine, however, has claimed the same in respect of physics, and virtually of the whole building of science — or at least natural science.

It is interesting to note that an important turn, maybe even a revolution is going on in the methodology of science. Historically, classical physics has played the role of ideal, rigorous science. Today, the tables are turning and a new ideal is being sought — namely, a science which is not purely constructive-hypothetico-deductive but

has a historical aspect as well, enabling us to accommodate irreversibility into scientific research. It is of course possible that physics can fulfil this task without any help from outside. Still, as we shall see more clearly below, it may need some assistance from chemistry. However, if chemistry cannot be distinguished from physics, there will be no difference anyway.

Chemistry and biology

It may sound a little unconventional, but we can still say today: “Biology is first and foremost a historical discipline, although partially it also makes use of hypothetical-deductive theories which are based on human constructive activity (experiment, or observation which should be considered a quasi-experiment).” (Näpinen 2001: 160)

There is an obvious difference between chemistry and biology. The latter deals with individual living beings and their populations, while the immediate object of chemistry is inanimate matter. The possibilities of experimenting seem to be more limited in biology than in chemistry. Evidently, we cannot do anything we’d like with living beings. However, there are strict limitations on what we can and what we cannot do in chemistry as well. Making up a list of these limitations is not the main philosophical interest here: it is a much more interesting task to find the reasons for the limitations. Trying to do this, we arrive at an astonishing result. It appears that the basis for the limitations on experimenting in biology and chemistry is fundamentally the same — namely, the irreversibility of all processes. We may carry through a similar chemical reaction for several times, just like we can breed several similar ducks. But the situations and circumstances are never exactly the same. Probably, exact sameness is not really necessary for scientific research. However, this is not at issue here. Nevertheless, in spite of this basic common limitation on experimenting, chemistry is clearly not biology due to the essential difference in the research objects.

Chemistry as a physics-like science

Chemistry has often been called a physics-like, or simply physical, science. Sometimes it has even been called the only experimental physical science beside physics itself. For instance, the late Edward F. Caldin (2002: 104) states: “The experimental physical sciences are physics and chemistry.” Moreover, Caldin does not hesitate to add (2002: 104): “Although these sciences (physics and chemistry — P.M.) have traditionally been distinguished, for *historical* and *accidental* (my italics — P.M.) reasons, it is hard to see that there is any fundamental difference between them.” Caldin sees only a difference of emphasis between physics and chemistry. He declares: “Chemistry is a quantitative science, based on measurement; it shares with physics both the analytical power and the limitations of the metrical approach.” (Caldin 2002: 105)

It is clear that Caldin’s position is not that of a superficial post-modern methodologist who generalizes furiously without looking seriously into the hard scientific core of his research object. Caldin recognizes the advantages of the quantitative approach which shaped modern chemical science, in contrast to the practices of mediaeval alchemists. Still, he thinks there is no fundamental difference between chemistry and physics.

The nature of laws in chemistry

Let us return to Caldin’s views once again. He specifies his position as follows: “The whole chemistry depends on our being able to isolate pure substances with reproducible properties.” (Caldin 2002: 110) If so, chemistry has a specific feature which is normally not attributed to physical sciences. Namely, we can say that physical sciences do not seek functional relations only. Sometimes they are interested in ‘natural kinds’ as well. Such considerations are based on the nature of laws in chemistry. There are laws stating that kinds of material with reproducible properties exist.

This observation is important for us as a point of difference between chemistry and physics. We can see that chemistry is really not just a part of physics in any sense but has the character of physics-likeness. At the same time, we have discovered some biology-likeness in chemistry, although the material kinds sought for in chemistry are quite different from the 'natural kinds' of biological classification.

In connection with the issue of laws in chemistry Caldin makes a further remark (2002: 110): "Such laws are always subject to correction; they do not attain certainty." On the face of it, this statement seems to refer to the Prigoginean idea of the end of certainty in science. But saying so would probably be a misstatement. What Caldin has in mind is rather a gradual movement towards precision never reaching finite certainty which is so common in science as a whole. There is no clear indication that Caldin has taken a methodological stand in favour of science being an uncertain business of explanation in principle. He is only stressing a typical feature of empirical laws — the idea that they are continually being improved and made more accurate, more specific and more precise.

Chemistry as the basis of the 'paradigm of uncertainty'

The late Ilya Prigogine presented the methodological approach, which we conditionally have named the 'paradigm of uncertainty' here, in his "The End of Certainty" (1997). The guiding idea of the paradigm is that imprecise results in scientific research are not due to deficit in human knowledge, but to the objective character of reality. On most occasions, it is simply impossible to get precise predictions due to certain problems with the representation of initial conditions. However, we can still make predictions, given some conditions. For instance, we can sometimes predict the shape of the attractor the system is entering. This is important since there can hardly be any science, even classifying-descriptive-historical science, if there is no possibility to predict.

Irreversibility is the crucial issue. If we admit irreversibility, then everything is unique. And it is very hard to predict what kind of uniqueness will appear next. However, another point is more important: recent developments in nonequilibrium physics and chemistry have shown unambiguously that the arrow of time is a source of order (Prigogine 1997: 26). Within the context of this paper it is essential to note that Prigogine draws no sharp line between physics and chemistry when evaluating the effects of irreversibility. He does not mention biology in this context, although the parallel should be even more obvious here.

Now we might ask: can we bridge the gap between natural and social sciences? Prigogine and many others have suggested some caution with this issue. Systems which include humans are quite different from natural systems, either inanimate or living. Luckily, our present topic does not press us too much for an answer to these questions since chemistry is certainly not a social science. Let us only remark that social systems are so different from natural systems largely due to the presence of minds in them — but mental processes may well be of chemical nature.

We can make one more interesting observation when studying the condition of matter. Prigogine (1997: 67) holds that matter at equilibrium is blind while matter far from equilibrium starts to see. In states which are far from equilibrium new processes set in and the production of entropy is increased. Prigogine reports of a steady progress in far-from-equilibrium chemistry, saying that in recent years nonequilibrium spatial structures (first predicted by Alan Turing in the context of morphogenesis) have been observed (Prigogine 1997: 67–68). Suddenly, chemistry has become a centrepiece of an emerging new paradigm in natural science. Prigogine himself, however, thinks that chemistry here is an accidental rather than a necessary example: “We have considered chemistry for the purposes of this discussion, but similar processes associated with nonequilibrium dissipative structures have been studied in many other fields, including hydrodynamics, optics, and liquid crystals.” (Prigogine 1997: 68) So, the specificity of chemistry is being questioned once again. Obviously,

those other branches of science that Prigogine lists here can easily be included into physics.

Conclusion

Chemistry does not fit very well into the same category with any other branch of natural science. It can be regarded as a constructive-hypothetico-deductive science, or as a classifying-descriptive-historical science. It can be viewed both as a ϕ -science and a non- ϕ -science. A typical ϕ -science constructs idealized objects; chemistry may do this but does not need to. Absence of this necessity is essential for breaking out of the bounds of classical science. In chemical research, we can take reality as it shows itself to us. Most important of all, chemistry enables us to accommodate irreversibility — which is so normal in everyday life — into science. It is much more easy to admit the fundamental impossibility of repeating experiments in chemistry than it is in physics. The need to include the observer into the system studied is usual in chemistry — in a discipline that produces new ‘stuff’ for itself. Production of new substances has to be guided by the observer-organizer. At least the observer has to create the conditions for self-organization which may lead in the necessary direction. Often enough, this is all we can possibly do in rearranging reality. It may even be dangerous to aim at anything more.

From the point of view of applications, chemistry, physics and biology often work hand in hand. For instance, physicists and chemists cooperate efficiently in manufacturing nanostructures. A unified chemical-biological approach is clearly needed in contemporary cognitive science, in the study of the functions of the human brain. This latter example suggests that the role of philosophy in the development of science may increase. However, by all evidence, it is going to be philosophy of mind, or general philosophy of (natural) science, which will play such a role — not philosophy of chemistry, physics, or biology.

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Concentric Patterns in the Brain: A Thermodynamic Aspect of Disease

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For the investigators of “Balo’s concentric sclerosis” (BCS) it was intriguing to find concentric patterns in the brain — first in the course of neuropathological examination, and subsequently on magnetic resonance images. Such patterns in the brain have also been observed in connection with some other conditions such as ischemia.

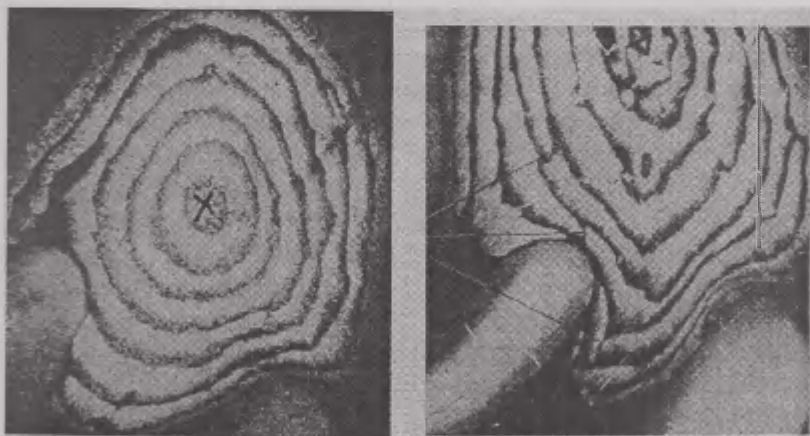


Figure 1. Microscopic examination of the brain of a patient with concentric sclerosis. The concentric pattern is similar to Liesegang rings. Parallel rings with a “storm” center (X) (Balo 1928) — left, distorted rings (Hallervorden and Spatz 1933) — right.

The neurological condition of concentric sclerosis was described for the first time in 1906. The pathologists of this time noticed a particular pattern in the brain. Balo (1928: 242–264), a Romanian neurologist after whom the disease was later named, wrote: “The concentric foci develop in such a manner that degenerated layers alternate with normal layers of white matter.” The causative agent proposed by Balo was a lecithinolytic ferment leading to demyelination. This factor was considered to act on the myelin sheaths and could be either produced locally or as a result of a disturbance in the internal metabolism or by an invasion into the brain’s white matter.

The non-specificity of the concentric patterns in the brain (Courville et al 1964: 1–6) invites one to view this phenomenon in the context of Prigogine’s theory of dissipative structures. Are we dealing with an oscillatory reaction which takes place in the brain as a medium? A survey of ideas involved in the experimental models of chemical self-organization and the theory of dissipative structures, together with the knowledge of the properties of lipids, may give new insights into disease.

Different kinds of patterns have been observed in nature for centuries. They inspired a German biologist from Goettingen, Johann Friedrich Blumenbach (1752–1840) to publish a paper (1780: 247–266) “Über Bildungstrieb (*Nisus formativus*) und seinen Einfluß auf die Generation und Reproduktion”. Blumenbach wrote: “About two years ago when I spent a vacation in the country I found in a water course by the flour-mill some kind of polyps.” The pattern of these creatures (zooids) which changed during the following days, and a man with deformities of the bones whom Blumenbach observed later, were the background for his theory of the “formation-drive” (*Bildungstrieb*). Blumenbach saw a connection between the patterns observed in the water and those resulting from the bone disease. He suggested that the “drive” was a general feature of bodies which formed the basic cause of generation, nutrition and reproduction. Blumenbach also differentiated this formation-drive from other powers of nature.

Later on, the notion of *Bildungstrieb* came to interact with Immanuel Kant’s (1724–1804) ideas; on the other hand, it went on to

greatly influence some idealist philosophers — in particular, Friedrich Schelling (1775–1854).

Kant (1987) accepted Blumenbach's notion of *Bildungstrieb* and developed it in his *Critique of the Power of Judgement*. Kant analyzed the question of understanding organic life in terms of the purposefulness of the structure and the function of living organism.

Beautiful nature contains countless things as to which we at once take every one as in their judgement concurring with our own, and as to which we may further expect this concurrence without facts finding us far astray. But in respect of our judgement upon the sublime in nature, we cannot so easily vouch for ready acceptance by others. For a far higher degree of culture, not merely of the aesthetic judgement, but also of the faculties of cognition which lie at its basis, seems to be requisite to enable us to lay down a judgement upon this high distinction of natural objects.

Kant also gave the background for later chemical experiments involving self-organizing systems.

(...) we have nature in its free formations displaying on all sides extensive mechanical proclivity to producing forms seemingly made, as it were, for the aesthetic employment of our judgement, without affording the least support to the supposition of a need for anything over and above its mechanism, as mere nature, to enable them to be final for our judgement apart from their being grounded upon any idea. The above expression, "free formations" of nature, is, however, here used to denote such as are originally set up in a fluid at rest where the volatilization or separation of some constituent (sometimes merely of caloric value) leaves the residue on solidification to assume a definite shape or structure (figure or texture) which differs with specific differences of the matter, but for the same matter is invariable. Here, however, it is taken for granted that, as the true meaning of a fluid requires, the matter in the fluid is completely dissolved and not a mere admixture of solid particles simply held there in suspension. The formation,

then, takes place by a concussion, i.e., by a sudden solidification— not by a gradual transition from the fluid to the solid state, but, as it were, by a leap. This transition is termed crystallization.

Schelling (1984) used the notion of *Bildungstrieb* as one of the prime forces he described in his *Naturphilosophie*. “To make the objective primary, and to derive the subjective from that, is, as has just been shown, the problem of naturephilosophy.” Schelling complains that Newtonian science is explanatorily vacuous and unable to account for the concepts it uses; it is incapable of comprehending the existence of self-organizing, organic beings, and deals only with possibilities.

Schelling indicated three powers or *Potenzen* (Pfau 1994):

- A1 — the lowest, acts as a kind of involution, [whose] principle ... is *Schwerkraft*,
- A2 — is activity, thus far only posited as implicit or as potential [but which] is now being posited as explicit or actual, namely, as the actual life of matter, that is as the dynamic process,
- A3 — in nature expresses nothing other than the supreme Being that has been elevated from nonbeing, that is, the innermost [core] of nature.

Schelling introduced a third force, *Schwerkraft*, into the system of Kant's dynamics which consisted of attraction and repulsion. According to Schelling's *Ideas for a Philosophy of Nature* (1988):

Force is simply that which affects us. What affects us we call real, and what is real exists only in sensation; force is therefore that which alone corresponds to our concept of quality. But every quality, insofar as it is to affect us, must have a degree, and that a specific degree [...]. But so long as we think of these dynamical forces quite generally — in a wholly indeterminate relationship — neither one of them has a particular degree [...]. All quality of matter rests wholly and solely on the intensity of its basic forces (*Grundkräfte*), and since chemistry is properly concerned only with the qualities of matter, we have thereby at once

elucidated and confirmed the concept of chemistry ... (as a science which teaches us how a freeplay of dynamical forces may be possible)... Chemistry is itself nothing else but applied dynamics, or dynamics considered in its contingency. [... It] considers matter in its becoming, and has as its object a free play.

In *Philosophical Inquiries into the Nature of Human Freedom* Schelling compares disease to evil. He described disease as a perturbation introduced into nature as a result of exceeded freedom. Disease is inseparably connected to hidden drives necessarily breaking out in its course. It develops in a particular part of the body because “something” designated to be a part of a whole starts to exist for itself. What is positive is always a whole, or forms a separate unit — the contraries to this are the breaking, disharmony and ataxia of forces. To cure disease one must build up anew the relations between the periphery and the center.

Friedlieb Ferdinand Runge (1795–1867), who was brought up in the atmosphere of *Naturphilosophie*, worked on the conformability of the chemical constituents of plants and their shape. In 1850 he published “Musterbilder” and in 1855 “Bildungstrieb” — two papers in which he described the color patterns he obtained on blotting paper when pouring onto it, one after another, solutions of different substances. He attributed the formation of these patterns (*Musterbilder*) to a particular power — *Bildungstrieb*, which was not related to magnetism, electricity or galvanism. In *Hauswirtschaftlichen Briefe* (1866) he wrote (Kuhnert and Niedersen 1999: 23):

The presented upper picture is my chemical arms. It was not created artificially, but in a natural way. Nor the pencil or the brush were used to draw the outlines and to fill it. No dye was used to colour in. Two colorless solutions were brought to interact on blotting paper and combine to form the picture. One looks at it against the light. There is no painter, even the sun is able to create something like that. I named the creating power forming these pictures as “formative drive” (*Bildungstrieb der Stoffe*).

Raphael Eduard Liesegang (1869–1947) was familiar with Runge's works. As an expert in colloid chemistry he worked with gels as a medium for chemical reactions. During his work in the photochemical company of his father he analyzed the physico-chemical basis of reactions in the outer layer of photopaper. This was the origin of the silver and chrome salts he used in later experiments. On the other hand, he studied the book by E. Kapp (1877) *Grundlinien einer Philosophie der Technik. Zur Entstehungsgeschichte der Cultur aus neuen Gesichtspunkten* (see Kuhnert and Niedersen 1999: 27). This book contained analogies between artificially created instruments and the natural organs of human beings (e.g. the hammer and the fist, musical instruments and the inner ear, the telegraph and the nervous system). Inspired by this, Liesegang too used analogies as a method in his experiments. Is a gel a peculiar aggregation state of human or animal organism? This was his question. Looking for an answer, Liesegang found that it is possible to reproduce organism-like patterns with the help of chemical reactions in gels.

As a natural philosopher and monist, Liesegang tried to give philosophical answers to questions which were not particularly rational. But later in his works he abandoned the imitation of organism-like structures in experiments and tried to explain phenomena by measurable factors, avoiding the introduction of occult determinants. For the first time Liesegang presented his work on patterns in gels in 1896 when he published a paper in *Naturwissenschaftlichen Wochenschrift* (Kuhnert and Niedersen 1999: 30). He observed that the diffusion of silver nitrate in a gel containing dichromate produced a concentric ring pattern. In 1906 he discovered rhythmic crystallization which he described in his paper "Geschichtete Strukturen". During the drying of this gel the saturation concentration is exceeded and this results in the formation of crystals. But the crystals do not precipitate in a uniform way; instead, they form a striping pattern.

The neurologists of the first decades of the 20th century were familiar with Liesegang's experiments. Among researchers studying concentric sclerosis, Balo, Hallervorden and Spatz were those who, in 1933, interpreted the pathology of the disease as a result of the physico-chemical phenomenon known as the Liesegang rings. Their

research revealed various periodic patterns — not only concentric rings, but waves and spirals as well. Hallervorden and Spatz (1933: 641–701) used thin blocks of fresh brain covered with a thin layer of potassium dichromate gelatin treated with silver nitrate.

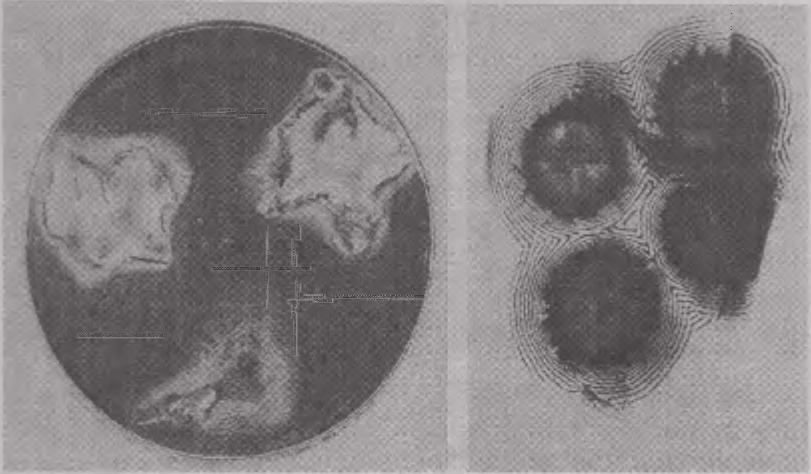


Figure 2. The experiment of Hallervorden and Spatz (1933). Thin blocks of fresh brain covered with a thin layer of potassium dichromate gelatin treated with silver nitrate. This experiment enabled to interpret the pathology of concentric sclerosis as a result of the physico-chemical phenomenon known as the Liesegang rings.

The mechanism proposed for the explanation of the Liesegang rings arises from Wilhelm Ostwald's ideas. Two main ideas were used: supersaturation and ripening (maturation) (Kuhnert and Niedersen 1999: 30–32).

In 1897 Ostwald proposed the supersaturation theory of the Liesegang rings. According to this theory silver nitrate forms a solution in the gel which is supersaturated with silver chromate. Precipitation does not occur until the metastable threshold is

exceeded. The area which is silver chromate depleted is due to the diffusion of chromate ions in the direction of the precipitate, so that the product of silver chromate solubility is no more exceeded. In some distant zone silver ions start to precipitate, and so the process is repeated. The supersaturation theory explains the growing distance of the rings from the center as a result of the gradually decreasing concentration of silver ions due to repeated precipitation leading to a delayed formation of the product of silver chromate solubility. However, this model did not answer the question why the concentration gradient of chromate ions in the gel is possible despite the diffusion of silver nitrate.

In 1900 Ostwald suggested a new idea which is discussed until today — Ostwald-ripening (maturation). This theory takes the precipitate as a starting point. Crystals of different size compete in the precipitate for growth. The bigger crystals grow faster than the smaller ones which leads to the depletion of particular ions in their environment. A concentration gradient will emerge and, as a result, the ions diffuse from the neighbourhood of smaller crystals in the direction of bigger ones. This leads to the shift of balance between the solid and soluble phase of small crystals due to the continuous removal of ions.

Crystallization in a medium with diffusion is a highly non-linear process where the local concentration of a chemical species is determined both by mass transportation (the concentration gradient) and by precipitation (local supersaturation). In these systems, the relaxation of concentration gradients produces local increases in the supersaturation. If critical supersaturation is reached at one such point, nucleation occurs, which depletes one or more of the reactants from the solution thus increasing the concentration gradient. In this way, a self-organized system is established in which the kinetics of mass transport and precipitation interplay to produce spatio-temporal patterns.

In these spatio-temporal patterns, the initial conditions (and the geometry of the system) will determine the kind of crystal distribution which is obtained: whether there will be no crystals at all, or a single jumble of microcrystals, or an amorphous precipitate, or other more interesting patterns like rhythmic bands or single crystals which are more or less evenly distributed. In the latter two cases, as a result of

the dynamics of pattern formation, the crystals which form the newer bands are of larger size and more perfectly crystallized. As suggested by Ostwald, and later elaborated through numerical simulation and experimental inference, these crystal distributions can be explained as due to a supersaturation wave travelling across the system as a result of the collective effect of different local precipitation events at different values of supersaturation.

Smith (1984: 3102–3103) reinterpreted Ostwald's supersaturation theory of rhythmic precipitation. He included "(...) nucleation, colloidal growth, and colloidal aggregation as intermediate steps in the production of visible precipitation rings." In this work the Ostwald "(...) theory [was] extended to arbitrary values of the initial concentration ratio, and ... used to predict its own domain of validity by regarding the ring spacing ratio and the fractional width of the rings as measures of the degree of difficulty of formation". According to Smith "the theory does not predict secondary banding effects or finite ring numbers which appear to exist in its domain of validity, but otherwise the predictions of the theory appear to agree with experiments (...)". He stated that "the Ostwald theory in its quantitative form can survive all criticism arising from the discovery of colloidal precursors provided (...)".

Mathematical formulations of the Ostwald mechanism were given by Prager (1956: 279–283) and by Zeldovich, Barrenblatt and Salganik (1962: 869–873). The later experiments of Flicker and Ross (1974: 3458–3465) suggested that the structures obtained (a uniform solution of KI and $\text{Pb}(\text{NO}_3)_2$) "(...) form by the autocatalytic growth of colloidal precipitate particles which, combined with diffusion of reacting ions, gives a morphogenetic instability of the kind suggested by Turing."

The English mathematician and logician Alan Turing examined in his work the *Chemical Basis of Morphogenesis* the first model of nonlinear interactions of the components in a system combined with transport processes. In 1952 he published a mathematical theory of structure formation in an initially homogenous system where chemical reactions occur simultaneously, including autocatalytic processes accompanied by energy consumption, and the passive processes of

transport-diffusion. Turing's ideas form the foundation of the modern theory of nonlinear systems, self-organization, and synergetics.

The equations presented by Turing are called the *reaction-diffusion equations*. In linear systems, diffusion is a process that leads to the equalization of concentrations over the whole reaction volume. But in the case of nonlinear interaction an instability of a homogenous stationary state can arise, and complex spatio-time regimes will emerge — like autowaves or dissipative structures. They are represented by a stationary, spatially homogenous distribution of concentrations, maintained due to the dissipation of the system's energy. The emergence of structures in such a system is determined by the difference in the diffusion coefficients of reagents, namely, by the presence of a short-range “activator” with a small diffusion coefficient and a long-range “inhibitor” with a large diffusion coefficient. Such regimes in a two-component system were examined in detail on the basic model of a “brusselator” developed in 1968 by Prigogine and Lefevre and named after the Brussels school of thermodynamics headed by Prigogine (Kuhnert and Niedersen 1999: 41–45).

The Turing structure is described and analyzed in *Modern Thermodynamics* by Dilip Kondepudi and Ilya Prigogine (1998: 445–447):

Diffusion usually homogenizes the concentration in a system, but when coupled with autocatalytic chemical reactions under far-from-equilibrium conditions, it actually generates inhomogeneities or patterns. For pattern formation, the diffusion coefficients must be different. If the diffusion coefficients are nearly equal, then diffusion does not cause an instability; diffusion only tends to homogenize the instability that already exists (...). For the emergence of spatial patterns, the diffusion coefficients must be *unequal*. In a small region, if one of the species diffuses out more rapidly than the other, the growth of one species may be facilitated by the depletion of the other. If it happens, the homogenous state will no longer be stable and inhomogeneities will begin to grow.

This is in concordance with Ostwald's explanation of the Liesegang rings. Structural instabilities are another kind of instability discussed by Prigogine (1998: 450–451). They

(...) arose in a given set of chemical reactions. In nonequilibrium chemical systems, instability may also arise by the introduction of a new chemical species which gives rise to new reactions; these new reactions may destabilize the system and drive it to new states of organization. In this case the "structure" of the chemical reaction network is itself subject to changes. Each new species alters the reaction kinetics and this may drastically alter the state of the system (..) which may (...) become unstable and evolve to a new state.

Each new structural instability generally increases the dissipation or entropy production in the system because it increases the number of reactions. This in contrast to the near-equilibrium situations in which the entropy production tends to a minimum. Structural instability may progressively drive far-from-equilibrium systems to higher states of entropy production and higher states of order.

Prigogine also wrote:

From the delicate beauty of the butterfly to the "fearful symmetry" of the tiger, Nature is full of wondrous patterns, both animate and the inanimate. How do these patterns arise? Dissipative process in systems far from thermodynamic equilibrium may provide at least a partial answer.

Prigogine (1998: 462) analyzes some examples of nonequilibrium thermodynamics.

After starvation some of the cells (*Dictyostellium discoideum*) begin to synthesize and release signals of a chemical substance known as cyclic adenosine monophosphate (cAMP) in the extracellular medium. The synthesis and release are periodic, just as in the chemical clock of the Belousov — Zhabotynsky (BZ) system, with a well defined period for a given experimental conditions. The cAMP released by the "pioneer" cells diffuses into the extracellular

medium and reaches the surface of the neighboring cells. Two types of events are then switched on.

First, these cells perform an oriented movement called chemotaxis toward the regions of higher concentration of cAMP i.e. toward the pioneer cells. This motion gives rise to density patterns among the cells that look very much like the wave pattern in BZ reagent.

Second, the process of aggregation is accelerated by the ability of sensitized cells to amplify the signal and to relay it in the medium. This enables the organism to control a large territory and form a multicellular body.

Thus the response to the starvation constraint gives rise to a new level of organization, resulting from the concerted behavior of a large number of cells and enabling an organism to respond flexibly to a hostile environment. (...) the process of chemotaxis leads to amplification of the heterogeneity formed initially, when the pioneer cells begin to emit pulses of cAMP. Because it enhances the density of cells near the emission center, chemotaxis enhances movement of the other cells toward it. This constitutes what one usually calls a feedback loop, very similar to chemical autocatalysis.

The conditions described above may be further linked to:

(...) a second feedback mechanism (...) operates at the subcellular level and is responsible for both the periodic emission of cAMP and the relay of the chemotactic signal. This mechanism is related to the synthesis of cAMP by the cell. The cAMP arises from the transformation of (...) adenosine triphosphate (ATP) which (...) is one of the principal carriers of energy within living cells. But the ATP \rightarrow cAMP transformation is not spontaneous; a catalyst [enzyme] is needed to accelerate it to a level compatible with vital requirements.

(...) many (...) enzymes (...) have (...) catalytic and (...) regulatory [sites]. When special effector molecules bind to the regulatory sites, the catalytic function is considerably affected. In some cases the molecules reacting with or

produced from the catalytic site may also act as effector molecules. This will switch on a feedback loop, which will be positive (with activation) if the result is the enhancement of the rate of catalysis, or negative (with inhibition) otherwise. The enzyme that catalyzes $\text{ATP} \rightarrow \text{cAMP}$ conversion is called adenosine cyclase and is fixed at the interior of the cell membrane. It interacts with a receptor fixed at the exterior phase of the membrane in a cooperative fashion (...). The resulting cAMP diffuses into the extracellular medium through the cell membrane and can bind to the receptor and activate it. In this way it enhances its own production, thereby giving rise to a feedback loop capable of amplifying signals and of inducing oscillatory behavior.

When considering concentric patterns in the brain characteristic of concentric sclerosis and ischemia one may find some parallels to the phenomena described by Prigogine. On the one hand, there is the diffusion of chemical components (e.g. phospholipids) in the medium of the brain, which eventually leads to the formation of concentric patterns, on the other hand, pulses of cAMP seem to be mechanisms involved in pattern formation.

The lipids, the main chemical constituents of the brain, may form dissipative structures under particular conditions. Gutberlet and Vollhardt (1995: 429–435) showed that monolayers of long-chain fatty acid esters (octadecanoic acid methyl ester, eicosanoic acid methyl ester, docosanoic acid methyl ester) develop morphological structures. The esters dissolved in *n*-heptane were spread on twice-distilled water, and after the evaporation of the solvent the monolayer was compressed and expanded. Heating-cooling cycles were performed after the compression of the monolayer to a fixed area. The evolution of well-defined circular condensed phase domains was achieved by a heating — recooling cycle. Images of the textures of the condensed monolayer phases were obtained using a Brewster angle microscope (BAM). The images showed the complex structure of the condensed phase as one of circular domains with numerous holes in them, which, in their turn, contained small condensed phase domains.

The effect of temperature was such that after compression the increase in temperature made the regions of condensed esters more fluid and, starting from 39°C, the monolayer transformed into a homogenous phase which was reached at 44°C. Circular domains were formed when cooling started from 38°C. Further cooling produced inner structures in the circular domains, slow domain growth, formation of a regular network and an increase in the inner diameter of those domains. These structures disappeared at 28°C.

The underlying mechanism proposed by Gutberlet and Vollhardt is qualitatively related to a nucleation-growth mechanism. Beside the condensed phase domains that coexist with the fluid phase of low density, random cellular structures appear in it which evolve into a two-dimensional network of boundary lines under the influence of the temperature gradient. The formation of two-dimensional nuclei is a function of the supersaturation of the homogenous fluid phase during the recooling of the system. Nucleation of a few molecules starts at the temperature where the critical value of supersaturation is achieved, caused by the thermal motion of the amphiphilic molecules of water subphase. Above the critical size, the nuclei of the condensed phase grow spontaneously. The cellular patterns within the phase of low density are accounted for by dissipative structures induced by temperature gradients. So again Ostwald's idea of pattern formation comes into play.

Since the brain contains proteins as well, the research of Juan Garcia-Ruiz and his coworkers (Garcia-Ruiz et al 2001: 152) should also be considered in a survey of the relevant experiments. They used microgravity protein crystallization. The reactor consisted of two chambers containing a protein solution and a precipitating agent solution connected by a plug filled with agarose gel. Once under microgravity conditions, the plug is rotated to connect the protein with the precipitating agent solution. Then they start to diffuse one against the other. The initial conditions of the system were set so as to force the first precipitation event to occur far from equilibrium.

High supersaturation (...) [was] created immediately after the opening of the plug separating the reactor chambers. The first precipitate (...) [was], therefore, a jumble of small and low

quality crystals (even an amorphous phase may form, depending on the initial conditions) at the interface between the rotatory plug and the protein solution. Its formation depletes the concentration of protein in the neighboring zones. As the salt diffuses ahead through the long protein chamber, a new precipitation event takes place, this time at lower supersaturation and at a slower rate of development of supersaturation. Iteration of this process provokes subsequent nucleation events along the protein chamber at progressively lower supersaturation, producing less crystals of larger size and higher quality. The maximum of supersaturation advances as a wave across the protein chamber at decreasing velocity. Its amplitude first increases and later decreases with time as it moves ahead, a pattern characteristic of the coupling between counter-diffusion and precipitation. The width of the wave increases with time while its velocity decreases, which explains the larger size of the crystals formed at later precipitation events: after a single crystal nucleates in a given location, its final size is a function of the residence time inside the moving wave, [that is] it depends on the width of the wave and how fast it moves across the protein chamber. Therefore, unlike classical protein crystallization methods, this non-equilibrium technique explores in one single experiment a large number of crystallization conditions.

The studies of Holmuhamedow and Evtodienko (1986: 342) were carried through with a thin, unstirred layer of mitochondrial suspension. The researchers observed spatial structures in different experimental conditions.

The results of this work indicated the dependence of pattern formation in mitochondrial suspensions on the state of the systems of ion transfer via the inner membrane. (...) it has been shown that the direction of ion transfer is of great importance for spatial structure formation [that is] the patterning occurs just in the case of the spontaneous efflux of ions from mitochondria preloaded with either potassium in the presence of valinomycin or calcium or strontium. Pattern formation induced by [these ions] (...) [was] also shown to

be suppressed by inhibitors of the respiratory chain or divalent cation accumulation in mitochondria. Therefore divalent cations seem to play an important role in the formation of spatial dissipative structures and the effect is exerted not only by the extramitochondrial concentration of ions but also by its changing during the process of spontaneous efflux because no patterns are observed during the energy-dependent accumulation of potassium, calcium or strontium. Such a complex interaction between the state of energy-dependent ion transporting systems of mitochondria and the process of spatial structure formation means that the patterning cannot be accounted for by the effect of hydrodynamic fluxes in the open liquid layer alone.

All of the experiments mentioned above were carried out in non-equilibrium systems and are therefore in concordance with Prigogine's idea of dissipative structures. If one considers the brain as a system which may be shifted by some environmental and/or intrinsic factors to a far-from-equilibrium condition, and if one also takes into account the involvement of autocatalytic reactions, concentric sclerosis may be interpreted in terms of thermodynamics.

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Understanding of the World and the Scientific Paradigm of Self-Organization

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1. Introduction

My paper will focus on the problem of cooperation between the human and physical understanding of the world. In other words, I will speak about the need to bridge the gap between modern physical sciences and the humanities described by Charles Percy Snow (1959) half a century ago. Not many authors have written on this topic. Ken Wilber (1996), for example, has spoken about a four-quadrant perspective on reality: a perspective which has internal-individual, internal-collective, external-individual and external-collective dimensions. In order to understand reality we must somehow integrate all these four quadrants and all the levels of their development. Cophorne Macdonald (2000), using Wilber's terminology, has written about *deep understanding* which he connects with wisdom. He states:

Wisdom, in all its varieties, strikes me as inherently integrative because it involves assessing the IT aspects of reality (the *exterior-individual* and *exterior-collective*) from especially helpful I-grounded (*interior-individual*) and WE-grounded (*interior-collective*) perspectives. Wisdom also leads to an upleveling of the I, WE, and IT realms. (Macdonald 2000: 1)

Macdonald begins with the following general observation about wisdom.

First of all, “words of wisdom” are not wisdom; they are words *about* wisdom, *pointers at* wisdom. Wisdom is internal, embodied by persons — and in a somewhat different sense, by cultures. Wise actions are external. Thus, even wise actions are not wisdom; they are effects of wisdom. Wisdom is multifaceted, and because no two people develop all facets in the same way and to the same degree, there are many flavors of wisdom. That said, in all its modalities wisdom is a perspective-based, interpretation-based, evaluative mode of cognition. Wisdom is not about facts *per se*, it is about the context-linked meaning of facts. It is about the significance of facts and their implications. (Macdonald 2000: 1–2)

C. Macdonald proposes “a two-element strategy for developing deep understanding: On the one hand, *go outward and acquire relevant intellectual knowledge*. On the other, *go inward and find self-knowledge and a quiet mind*.” (Macdonald 2000: 4) In the Summary Macdonald adds:

It is suggested that we intellectually acquire knowledge of the sciences of energy, complexity, and information; systems and the evolutionary process; consciousness and the workings of the human brain/mind system; human cultures; economic systems; ethics and techniques for changing ethical perspectives; probability as a decision-making tool; the techniques of conflict resolution and effective persuasion; and what people are proposing and doing to solve the problems that the world faces. Regarding self-knowledge and the development of a quiet, receptive, Taoistic approach, it is suggested that we involve ourselves with mindfulness meditation and, at some point, Dzogchen practice. (Macdonald 2000: 6–7)

Dzogchen is a nondual practice, the aim of which is just TO BE, “and realize that your deepest, truest self is nothing other than this primal sentient-active oneness.” (Macdonald 2000: 6)

I have written on the topic of the relationship between the human and physical understanding of the world in connection with Prigo-

gine's paradigm of self-organization in several papers (Näpinen 2001a, 2001b, 2002, 2003, 2004, Näpinen and Mürsepp 2002). In the present article, I will especially consider the novel aspects in the world-view suggested by modern physics and chemistry. This new world-view differs radically from the understanding of the world implied by traditional mathematical natural science. During the last decades revolutionary changes have occurred in natural sciences, first of all, in physics and chemistry. The new phenomenon of self-organization has been discovered. The new aspects have been philosophically discussed by scientists studying self-organization themselves. In my paper, I shall especially concentrate on those discussions.

2. The concept of self-organization

In my view (see Näpinen 1993) the concept of self-organization is opposed to the concept of organization. The concept of organization denotes a process that leads to the rise of goal-oriented structures due to conscious human goal-directed action, or due to some external ordering influence. As to the concept of self-organization, it denotes a process that leads to the rise of goal-oriented structures without conscious human goal-directed action, or any external ordering influence. True, external factors are indispensable for self-organization, but only as conditions, not as ordering forces.

Historically, the beginnings of the concept of self-organization may be found already in Aristotle's doctrine of causality. Aristotle's four kinds of causes — *material, formal, efficient, and final causes* — I interpret, in their inseparable unity, as a philosophical concept of self-organization (embracing both the process without an external organizer, and its result). The first three kinds of causes I interpret as a philosophical concept of organization (involving an external organizer, the process and its result). The essential characteristic of a self-organizing system is its autonomous purposive behavior. The characteristics of a self-organizing system cannot be constructed

according to an external purpose. I note here that my understanding of the concept of self-organization and organization is close to Rein Vihalemm's view (see Vihalemm 2001). It must be stressed that theories, characterized as organization, are "dealing with the typical impact of the non-Aristotelian effective cause (instead of Aristotle's third cause) that realizes the external purpose, while Aristotle's natural final cause is ignored." (Vihalemm 2001: 194)

3. Self-organization: physics and chemistry

The concept of self-organization lies at the center of a larger theoretical revolution in physics — the belief that the fundamental laws of nature "describe a world which demands to be understood in a historical manner" (Prigogine 1998: 2). The main figure among scientists representing this belief has been Ilya Prigogine (1917–2003), who worked on nonlinear, nonequilibrium thermodynamics of chemical reactions and, in particular, on *dissipative structures*. To Prigogine, irreversibility is a fundamental property of physical systems. In a new microscopic equation, Prigogine (1980) combined the reversible and irreversible aspects of physical evolution.

Let us look at what Prigogine and some other scientists have said about the new physical world-view and about the new science of nature. Prigogine has written:

Over the past several decades, a new science has been born, the *physics of nonequilibrium processes*, and has led to concepts such as *self-organization* and *dissipative structures*, which are widely used today in a large spectrum of disciplines, including cosmology, chemistry, and biology, as well as ecology and the social sciences. ... Irreversibility can no longer be identified with a mere appearance that would disappear if we had perfect knowledge. Instead, it leads to coherence, to effects that encompass billions and billions of particles. ... We are actually the children of the arrow of time, of evolution, not its progenitors. (Prigogine 1997: 3)

Prigogine has also declared: "Mankind is at a turning point, the beginning of a new rationality in which science is no longer identified with certitude and probability with ignorance." (Prigogine 1997: 7) Why Prigogine chose to call the new kind of systems "dissipative structures", he explained as follows:

I wanted to bring together two concepts: the idea of structure, which generally is static; and dissipation, for which you need energy continually brought in and going out. This is the type of structure that may appear at some distance from equilibrium. Far from equilibrium you have specificity. The world is multiple: We have ants, elephants, plants, and civilizations. New, highly specific solutions appear when you go far from equilibrium. (Prigogine 1983: 17)

Convection cells, autocatalytic chemical reactions, and living systems are all examples of far-from-equilibrium dissipative structures which exhibit coherent behavior.

The next quotation from Agnessa Babloyantz specifically deals with the new chemistry and its object of study:

The twentieth century has witnessed a turning point in the chemical and biochemical sciences. New chemical reactions were discovered exhibiting unexpected properties and requiring new concepts for their understanding; a *new chemistry* was born. ...

In order to see, measure, and understand this new chemistry, we must do away with the idea of matter as something static and consider it in a dynamic framework. Matter and energy must flow continuously, chemical reactions must never stop, and thermodynamic equilibrium must be avoided at all cost. In such an environment, atoms and molecules cooperate, sometimes at the scale of the entire system, and produce bulk properties that could not be suspected from the behavior of the molecules and atoms. (Babloyantz 1986: 139)

During the last couple of decades, it has become common to speak about chemical becoming, chemical chaos and chemical self-organization (see Earley 1998, Salmon 2003). Joseph E. Earley has written in one of his articles:

Historically, important philosophical discussions of becoming (including those of Aristotle, Kant, Hegel, and Peirce) considered phenomena and entities that are now squarely in the province of chemistry. Chemists are interested in wholes and parts, in connections between features of components and properties of composite entities made up by those pieces. (Earley 1998: 105)

Earley considers two examples of chemical becoming: 1) 'van der Waals molecules' and 2) transition from chaos to coherent behavior in open chemical systems far from equilibrium. I will briefly survey the conceptual context of the second example.

Chemical reactions of the Belousov-Zhabotinsky type (i.e. the cerium ion-catalyzed oxidation of malonic acid by acidified bromate) can be carried out in continuously stirred tank reactors to which reagents are continuously supplied and from which products are continuously removed. Earley describes this experimental situation as follows:

The state of the contents of such reactors can be monitored by electrical or optical sensors. Under some conditions, the output of the monitoring device varies wildly and in an erratic manner. The pattern of readings in a given time interval *does not repeat*, no matter how long the system is observed. In such cases, it is *not possible* to predict the reading of the sensor at a future time on the basis of information (no matter how precise) on the state of the reactor at a particular time. This condition is called *chemical chaos*. (Earley 1998: 108–109; author's italics.)

The Belousov-Zhabotinsky reactions demonstrate the emergence of chemically self-organizing collections of processes. Such collections are called "dissipative structures" (in Prigogine's sense). According to Earley (2000), the coherence in these structures is defined by the

peculiar *closure* of the sets of relationships between the structure's components. Earley (2003a, 2003b) has demonstrated that, in order to deal adequately with open chemical systems, it would be useful to develop a new *mereology* (the philosophical study of wholes and parts). In dissipative structures parts (which in chemical dissipative structures are concentrations of the components of the system) are modified by their composition into a whole. The existing versions of mereology rely on the assumption that parts are not changed by being associated into wholes.

4. Self-organization: biology and history

Some changes in the overall understanding of the world are also manifest in biology. Prigogine (1997: 161–162) quoted Stephen J. Gould's definition of the historical character of life:

To understand the events and generalities of life's pathway, we must go beyond principles of evolutionary theory to a paleontological examination of the contingent pattern of life's history on our planet — the single actualized version among millions of plausible alternatives that happened not to occur. Such a view of life's history is highly contrary both to conventional deterministic models of Western science and to the deepest social traditions and psychological hopes of Western cultures for a history culminating in humans as life's highest expression and intended planetary steward. (Gould 1994: 84; quoted from Prigogine 1997: 161–162)

To this Prigogine responded:

We are in a world of multiple fluctuations, some of which have evolved, while others have regressed. This is in complete accord with the results of far-from-equilibrium thermodynamics. ... But we can now go even farther. These fluctuations are the macroscopic manifestations of fundamental properties of fluctuations arising on the microscopic

level of unstable dynamical systems. The difficulties emphasized by Gould are no longer present in our statistical formulation of the laws of nature. Irreversibility, and therefore the flow of time, starts at the dynamical level. It is amplified at the macroscopic level, then at the level of life, and finally at the level of human activity. What drove these transitions from one level to the next remains largely unknown, but at least we have achieved a noncontradictory description of nature rooted in dynamical instability. The descriptions of nature as presented by biology and physics now begin to converge. (Prigogine 1997: 162)¹

To the classical, dualistic world-view Prigogine opposed a new, nondualistic view:

The classical view divided the universe between spiritual self and the physical, external world. Yet inside us we see time, activity; we experience change. This internal experience is in complete contrast with the view of the world as a timeless automaton. As we begin to discover the roots of time outside us, this duality tends to disappear. We see a convergence between the world outside and the world inside us. With the paradigm of self-organization we see a transition from disorder to order. In the field of psychological activity this is perhaps the main experience we have — every artistic or scientific creation implies a transition from disorder to order. (Prigogine 1983: 16; italics by me. — L. N.)

¹ In this passage, Prigogine referred to his work which incorporated irreversibility into microscopic physics (1980). On the microscopic level of physical description Prigogine's theory deals with (mechanical and quantum) *large Poincaré systems*, which Prigogine identified with probabilistic imaginations irreducible to detached trajectories or detached wave functions (see e.g. Prigogine 1997: Ch. 5–6). These entities function as mathematical abstractions at the so-called *thermodynamic limit*: the number of particles and the volume in which the particles are located are approaching infinity, but the ratio of their number to the volume remains finite and constant. These entities have a continuous spectrum. Prigogine (2003) considered chemistry as belonging to the class of nonintegrable (i.e. with particles in incessant interaction) Poincaré systems.

Self-organization, indeed, is a notion, which comes from our everyday experience (Zwierlein 1994) and does not fit the ideal of exact description and prediction. From the viewpoint of philosophy the notion of self-organization can be associated with the individual and social-cultural self-interpretation of human beings who try to acquaint themselves with the world they live in. This self-interpretation is based on people's self-experience and self-cognition. The conceptual scheme broadened by Prigogine contains the element of *history* as an unconditioned component: the emergence of novelties is connected with irreversibility, events that can be described only through probability, and with changes in the pathways of the integral process of development caused by some events. This brings into physics the "narrative" element that so far worked only in historical sciences. With his paradigm of self-organization Prigogine has managed, at the theoretical level, to adjust the natural-scientific approach to the humanities.

To the interviewer's question 'What was the classical response to time-dependent processes?' Prigogine answered:

To try to avoid them. You see, the famous entropy principle isn't a real law. It simply states that some events are more likely to occur than others, since entropy is considered to be only an approximation. But because there was such a distrust of time, there was also a distrust of life, because all life is obviously time-oriented. Still, you will find many people saying that life is an accident — that life is not within the laws of physics. (Prigogine 1983: 16)

About the influence of the new science on the overall understanding of the world, Prigogine said:

Clearly, in the physical universe four types of phenomena occur. Structures appear, as with biological systems and social systems; and they disappear, as when you mix two liquids. There are also deterministic processes, like the motion of the earth around the sun, and nondeterministic processes. *What has changed is the perception of the relative importance of these processes.* We begin to see now

that the deterministic processes can be seen only in isolated, artificial systems. *The natural world, on the other hand, is a world of irreversible processes, of self-organization.* So I talk about a new dialogue with nature because I think *we are beginning to perceive nature on Earth in exactly the opposite way we viewed it in classical physics.* We no longer conceive of nature as a passive object. I can't stress enough that it is an active object in our lives. And we see now that life has much deeper roots than we once suspected. (Prigogine 1983: 16–17; italics by me. — L. N.)

So, Prigogine insists that outside isolated, artificial experimental situations processes contain an essential element of chance and irreversibility. In these situations, the world can no longer be observed as something passive (as it was in classical science), but it is understood as something characterized by spontaneous activity. Only in the conditions of an experiment (and quasi-experiment) phenomena can be *nearly* reversible and *nearly* necessary.

Of course, as Darwin would not have discovered natural selection if he had known nothing about artificial selection, so Prigogine would not have discovered self-organization in physics and chemistry if he could not base his thinking on his knowledge concerning artificial situations — like investigations of the Belousov-Zhabotinsky type of chemical reactions. Darwin and Prigogine have, surely, dealt with different aspects of nature. The concept of natural selection means that the environment chooses stronger individuals. The concept of self-organization means that elements of spontaneous development create self-organization (the same set of boundary conditions may give rise to different dissipative structures). Natural selection has external causes, self-organization is completely determined by inner causes. The former concept stresses competition, the latter emphasizes cooperation. Stuart A. Kauffman (1993, 1995), one of the leading figures in the study of self-organization and complexity nowadays, has pointed out that the evolution of the whole world appears to be a combination of selection and self-organization. Thus the understanding of evolution by natural selection is incomplete. Or, as Prigogine recently noted: “It is now generally admitted that biological

evolution is the combined result of Darwin's natural selection as well as of self-organization which results from irreversible processes." (Kondepudi and Prigogine 1998: xii)

When speaking about self-organization in biology, one should also mention Manfred Eigen's theory of the self-organization of biological macromolecules (1971) which is based on Prigogine's nonequilibrium thermodynamics. The chances of such a theory the Russian chemist Alexandr P. Rudenko (1976) not long ago considered extremely limited. I have discussed this question in more detail in a previous article (Näpinen 1984). Eigen's *hypercycles* (self-reproducing cycles of catalytic and autocatalytic chemical reactions) are an example of Prigogine's dissipative structures. At first, Eigen allowed for the possibility that complexification (the emergence of life) starts with simple systems, but later he became convinced that complexification is not possible in simple systems; instead, *initially* complex systems may become more and more complex in the course of time (Eigen 1993). Kauffman (1995) also rejects the idea that life began with simple catalytic cycles.

To return once more to the larger framework of Prigogine's paradigm, the scientist's work, then, is a historical dialogue between a human being and nature. From the scientist, it requires the application of mathematics and experimentation. As for nature, this means that nature is not a passive performer of the scientist's expectations, but reality characterized by internal activity, unverifiability, unpredictability, etc. — reality that presents challenges to the scientist. The scientist's work should be understood as mutual activity between the human being and nature, where nature generates problems and the scientist tries to solve them. As for the religious implications of this attitude, Prigogine has said the following:

"I think that ... the duality ... — between seeing the universe as an automaton or, on the other hand, as the picture of a guiding God who acts through us and has created both a dead universe and the human soul — is mistaken. I see us as nearer to a Taoist view, in which we are embedded in a universe that is not foreign to us." (Prigogine 1983: 25)

5. New natural science and laws

Thus, to my mind, one has good reason to claim that Prigogine's project invites us to remake (at least to some extent) the whole mathematical natural science into something what we, following Prigogine himself (Prigogine and Stengers 1977: Part 2) might call "a human science of nature". Prigogine has considered the physical activity as a process of creativity and innovation. Therefore the methods of cognition even in the physical-mathematical sciences cannot remain the same. Prigogine has recently explained his creative attempts at remaking physics in the following way:

On the scientific side, our project is perhaps to build a kind of theoretical structure that serves to *unify* rather than alienate man from nature. As a theoretical physicist I want to see what the rules of unification are. But unification also requires a better understanding of diversity. Once we see *chaos* as playing an essential role in the basic laws, we see that the basic laws are probability laws, and from there a whole spectrum of possibilities emerge.

In my work I am trying to draw a more unified picture of our universe, and *at the same time I am attempting to define our universe as temporal, pluralistic and complex.* That is already a big project! (Prigogine 1999–2001: 7; italics by me. — L. N.)

As already indicated above, in the Newtonian mechanical paradigm nature is separated from man and considered inert. In contrast, in the new scientific paradigm (Prigogine 1980, 1997; Prigogine and Stengers 1984) nature is self-organizing and includes humans. Prigogine has compared the new conception of nature and the traditional physics of laws in the following way:

... The fundamental laws of nature, as usually formulated, in classical or quantum terms, define an ideal intelligibility, that of the demon of Laplace or of Maxwell. However they raise the problem of what these demons cannot see: that approach would render them incapable of raising the

problem of the *qualitative* difference between the behavior regimes of matter, incapable of studying *nature as combining order and disorder, regularity and chaos, the repetitive and the new. ...*

To consider the fundamental laws of physics in irreducibly probabilistic terms is to radically change their meaning. They then designate not certainty but possibilities as the ultimate mode of physical intelligibility. Must we regret it? ... I would much rather think that the Universe is constantly evolving, like nature, like man. The new formulation of the laws of nature, which combines the notions of law and event, affirms their coherence.

The meaning of the laws of nature is therefore profoundly altered, at the level of their fundamental, dynamic formulation. The possibilities they then express no longer allow for reference to a fuller description, which would be a deterministic description. Furthermore, the time symmetry is broken: future and past cease to play equivalent roles. The laws of nature describe a world which demands to be understood in a *historical* manner. *The physics of the laws thus opens itself in a coherent way to the notions of events and novelty without which what we call nature would be incomprehensible.*

Until recently the conception of nature put forward by physics placed the stress on stability and equilibrium. Biology and human history therefore seemed "abnormal", remote from the "normal" behavior attributed to matter. Today we see instability, fluctuations, irreversibility at every level.

The denial of time ... makes us strangers in the world we are trying to understand. ... We live in an open universe, the future is uncertain, but we can help to build it. (Prigogine 1998: 1-2; italics by me. — L. N.)

As we see, on Prigogine's interpretation, the understanding of nature is not reduced to the subordination to laws any more. The denial of time as irreversibility is always a denial of reality. For Prigogine a

scientist is not a fiction, not a Cartesian thinking substance relying on mathematics: rather, it is a biological, social and historical being. The scientist no more studies the world from an absolute viewpoint (which could be ascribed to God or at least to a demonic mind) but poses problems, determines the framework in which the problem has a meaning, chooses the method of description, etc. Scientific description cannot any more be separated from an actual scientist and attributed to an omniscient being for whom everything particularly characteristic of the human world (chaos, irreversibility, instability, indeterminacy, chance, unpredictability, quality, events, novelty, temporal and spatial nonuniformity, historicity, etc.) is unreal.

I have pointed out earlier (Näpinen 2001a) that the paradigm of self-organization is part of new mathematical natural science which involves irreversibility and chance (randomness). This science formulates laws of a *new type*, which are at least to some extent in accordance with the open, evolving world including humans. Prigogine has considered the role of chance (randomness) in the new science to be no less important than that of necessity. This is shown by his own words: "... we can *never determine* when the next bifurcation will arise." (Quoted from Toffler 1984: xxxii; italics by me. — L. N.) It is important to realize that the far-from-equilibrium conditions created as a result of successive instabilities, as well as the practical infinity of a number of incessantly interacting system's units that guarantees the coherence of processes, Prigogine has regarded as the two fundamental characteristics of the *living* nature, and he has included these characteristics into the initial position of theoretical research of the physical world (Vihalemm and Näpinen 1987: 27).

Biological concepts or biological modes of thinking had not been used in mathematical physics prior to Prigogine. On the contrary, attempts were made to explain the origin and development of life, and even of human society, with the help of physical theories based on Newtonian principles. Prigogine, however, has tried to explain physical and chemical phenomena with the help of principles which were considered typical of living nature only. Moreover, the historical approach considered by Prigogine originates from disciplines which describe human history.

In my (Näpinen 2002, 2004) and Rein Vihalemm's (1995) opinion even the introduction of human concepts into physics by Prigogine is justified, but only if we take into account the limitations of both the classical and nonclassical exact sciences. In fact, Prigogine's approach is a cooperative enterprise, which tries to combine the classifying-descriptive-historical approach and the constructive-hypothetical-deductive method — and the first type of inquiry is the starting point. *The nonclassicalness of Prigogine's theories lies in the fact that these theories, for the first time in the history of exact sciences, explicitly take into account the history of systems and their self-organization.* It is exactly this what makes these theories “nonclassical” in the complete sense of the word, because the “classical” exact sciences (including quantum mechanics) are grounded on the idealization of reversibility of fundamental processes (Näpinen 1983).

At the theoretical-physical level, Prigogine started with a new interpretation of the second law of thermodynamics. According to his reading (which corresponds to Max Planck's) this law essentially claims that there is a quantity in nature which, through all changes occurring in nature, changes only in one direction (Prigogine and Stengers 1984: Ch. 8, §1). From this the important conclusion follows: if there are quantities in the world that change in only one direction, there are also states which change in one direction only (Prigogine 1980, Prigogine and Stengers 1984).

The traditional (statistical) interpretation of the second law of thermodynamics allows movement in the opposite direction as well; it merely considers its probability to be very small. *This conclusion about the existence of time-oriented states differs in principle from the idealized picture of traditional physics* where the initial conditions corresponding to some state of the object are arbitrary and not theoretically defined (Vihalemm and Näpinen 1986, 1987, Näpinen 1993). A theoretical meaning is given only to the equation expressing the laws that link the arbitrary initial conditions with the final result. But Prigogine has shown, in the language of mathematical science, that the real situations are oriented in time, that states and laws are closely connected with one another, that the initial conditions of the system emerge as the result of its previous evolution. Although under

certain conditions stable, reversible systems also exist, they must not be regarded as more fundamental than systems that are unstable to a remarkable extent. According to Prigogine, instability is closely linked with irreversibility: the irreversible, oriented time can emerge only because the future does not exist in the present.

Therefore we may say that, with the inclusion of the arrow of time and of the corresponding biological schemes, physics and chemistry will bring scientists closer to the understanding of nature: *the researcher becomes united with nature not by measuring or calculating the so-called initial conditions, but by investigating in what kind of systems and in what kind of conditions self-organization emerges*. In doing so researchers must remember that since self-organization is a phenomenon with intrinsic purposiveness (characterizable by Aristotle's final cause), self-organizing systems cannot be constructed by an external source. The results and conditions of the self-organizing processes are not predetermined. In all cases self-organization arises from the strongly nonequilibrium (creative) chaos which may be understood as a field of possibilities in the fundamentally indeterminate historical reality (Näpinen 2002: 133–135). Only the investigation of the various *kinds* of systems and the various *kinds* of conditions under which self-organization emerges can make it possible for human beings to participate in the natural-historical processes of endless generation and change. If a man wants to realize his goal he must unite his action with a self-organizing natural process, i.e. he has to participate in the self-organizing process of the whole world.

6. Concluding remarks

To my mind, the most important contribution of Ilya Prigogine is the inclusion (through irreversibility) of the chance factor in the understanding of the cosmos (Näpinen 2001a, 2002, 2004). In Prigogine's paradigm of self-organization, no two-worlds-problem (the human *versus* physical universe) exists any more. The idea of two separate

worlds — the human world and the physical universe — is replaced by the idea of one active, self-organizing world which includes humans with their organizing activity and its products. From now on natural science has ceased to strive for absolute truth, for certain knowledge achievable by mathematical means; instead, it is trying to achieve probabilistic knowledge, which unites the regular side of nature with its chaotic aspect. The new natural science accepts creativity which is based on chance and irreversibility in nature, and it also acknowledges the fundamental indeterminacy of the whole history of nature and of human society. Prigogine's new dynamic description requires a decisive abandonment of the level of fundamental description which is supposedly independent of the scientist. The scientist himself and his activity together with its products can now be treated as part of nature. Nature is understandable as a living being "who, thanks to the conceptual and technical idealization, is indeed predictable, even transformable and manipulable, but only locally, partially and relatively" (Prigogine and Stengers 1977: Part 2, 650).

Prigogine has tried to restore the conception of the unitary material world on the basis of the notion of *becoming*: he has tried to understand the world and the human being inside it as interrelated processes of becoming (emergence, change and disappearance). One of the reasons for Prigogine's success is the factual combining of the constructive and the historical approach. The constructive method is based on mathematical and experimental activity: it can describe and manipulate some of the regularities. The historical approach, based on analogies, is classifying and qualitatively descriptive, since it deals with phenomena that contain unique events and cannot be reduced to regularities. There is no need to try to create a new theory in order to understand unique events. Therefore, from now on even physics is an intellectual "mixture" which contains both the constructive basis and the natural-historical inquiry.

From recent scientific studies on self-organization we learn that, as in Chinese philosophy's vision of nature, we have to acknowledge the importance of the processes of generation and change. The cosmos is filled with the creativity of the process of endless transformations, and

human creativity derives from the creativity of the cosmos itself. Human constructive activity is justified indeed — but not a dominative construction. Instead, it has to be participative construction. As Vaclav Havel (1994: 4) has said: “... We are rooted in the earth and, at the same time, in the cosmos. This awareness endows us with the capacity for self-transcendence.”

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