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Technologies of the Future: Catalysis

“Die katalytische Kraft scheint darin zu bestehen, dass bestimmte Körper durch ihre bloße Gegenwart die bei dieser Temperatur sonst nur schlafenden Verwandtschaften zu erwecken vermögen.”

J. J. Berzelius (1779 – 1848)

Katalysatoren sind “... solche Stoffe. Durch deren Gegenwart langsam verlaufende Reaktionen beschleunigt werden.”

Wilhelm Ostwald (1853 – 1932)

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Summary

No other technical principle combines economic and ecological values as closely as *catalysis*. The inevitable plethora of manufactured products in advanced, industrialized societies will only be technically, economically and ecologically possible in future when valuable commercial products are produced, surplus products are degraded, and pollutants are avoided with the help of specific catalysts. Examples include the specific production of stereochemically pure pharmaceutical agents, the construction of tailored polymer materials from simple precursors, the degradation of no longer useable plastics as well as the reduction of pollutants from manufacturing plants and combustion systems (e.g., motor vehicles, power stations). Technical advances in the production, storage, and conversion of energy – another major topic for the 21st century – will also be promoted by catalysis research, as illustrated already by fuel cell technology. In view of the world market for catalysts of more than

US \$10 billion, with an increasing tendency, it is incomprehensible that Germany has not yet recognized the chances for a *national focus on catalyst research*. The structures for catalysis in Germany are still primitive. Even so, in no other place in the world is the potential for innovation better than in Germany, the country in which catalysis was originally discovered. Guarantees for success would be the many years of experience in industrial catalytic processes (e.g., ammonia synthesis, olefin polymerization, ethylene chlorination, hydroformylation), highly differentiated intermediate and fine chemical industries, numerous university and Max-Planck institutes with a proven record of success in homogenous and heterogeneous catalysis, as well as an excellent convergence of chemical-material and process technological expertise. Without parallel in the world, the prerequisites are available in Germany to realize advances in process development from molecular catalysts through their mechanisms of action to industrially relevant production systems by combining basic and applied research. It is today common practice that the further development and differentiation of the material world, irrespective of whether common consumer products, intelligent materials, or multifunctional drugs are concerned, depends on catalysts with ever increasing specificities. The industrial mimicking of natural models (biocatalysts) will also be of importance and commercial value. Catalysis is the ecological science with the largest economical potential.

Introduction: The Nature of Catalysis

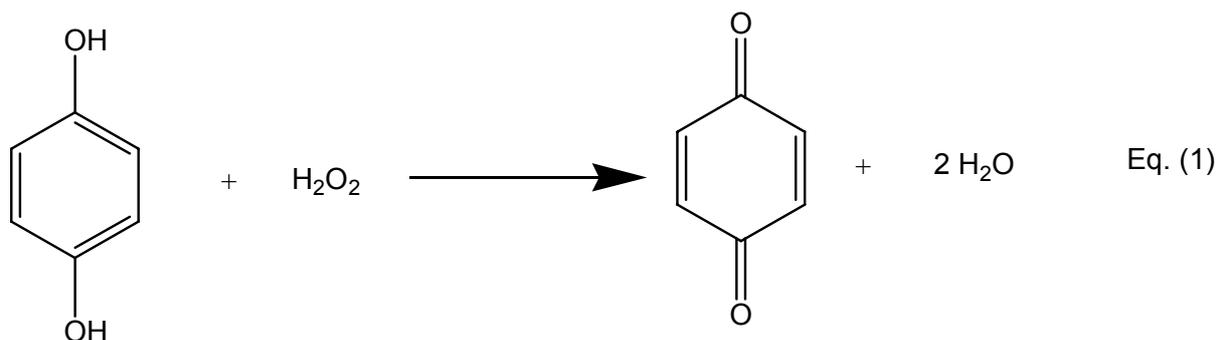
Catalysts are (chemical) individuals that, in the ideal case, are *specific in their action*, *highly active*, and have *long useful lifetimes*. The specific activity encompasses *regio- and stereoselectivity*, this means that, in a chemical reaction for synthesis or transformation, the catalyst selects specific binding sites (constitution) and at the same time allows only a particular spatial arrangement (conformation, configuration). Control of merely the constitution may be sufficient for simple molecules such as, e.g., the oxidation of ethylene to ethylene oxide or acetaldehyde. On the other hand, the synthesis of typical *life-science* products involves an additional high steric requirement that is normally only fulfilled by catalysts with a tailored spatial structure. It is just this distinction between the mere linking of atoms or groups and the precise spatial order (stereocontrol) that recommends catalysts as highly intelligent tools for the design of the material world¹⁻⁷.

Catalysts are (chemical) individuals that accompany a catalytic process by having a major, even decisive, influence on its course without themselves undergoing any change thereby. Catalysts thus have a secure identity. Accordingly, catalysts are not without a profile; on the contrary, a special *reaction profile* in combination a *steric profile* is the essential condition in order that other substances can meet at the active center to join together or to undergo other transformations. The better the fit for the reaction partners involved, the more specific is the action of the catalyst. The lifetime of the catalyst, as the period in which it expresses its specific activity, depends on whether it emerges intact from each reaction unit (catalyst cycle), i.e., whether it has retained its original structure and reactivity characteristics. The expert describes the degree of activity of a catalyst as its *turn over number* (TON) while the catalytic efficiency is described as the *turn over frequency* (TOF). Today, a complex pharmaceutical precursor requires a TON in the range 10^3 to $2 \cdot 10^5$. This means that one unit amount of catalyst (mol) produces the corresponding number of mols of product. In the case of TOF (in h^{-1}) this productivity is referred to the unit of time. The nature of catalysis can be reduced to an energy profile diagram (Fig. 1) that clearly reveals the energetic advantages.

In daily life we often hear that *something is catalyzed* or that *someone must act as a catalyst*. Even persistent catalysis is mentioned when a complex process must be kept in motion. It is always people, individuals with special talents, who bring others together and ensure that progress is made. And we know how important the results of such an activity can be. Although the major company mergers of today require analysts they do not make any progress without catalysts either at the start or during creation of the new company philosophy. The same is true for politics, nothing happens without catalysts whereas with catalysts the chemistry works.

Catalysts: Protagonists of Change

Catalysis is ubiquitous. It is exemplified by life since the very beginnings of life. There is hardly any biological process that can proceed without its catalyst, if only to ensure reaction specificity, in other words to maintain the variety of life. The best known biocatalysts are the *enzymes* which, depending on their function, are employed by nature in metal-free or metal-containing forms. Most essential metals, for example, zinc, are components of enzymes and function therein as reaction centers, but they also influence the structures of the enzymes themselves. This shows once more just how important the spatial structural arrangement of a catalyst is for its activity. One interesting example from nature is the defense and survival strategy of the bombardier beetle (Fig. 2). Under its stable chitin shell *Brachynus explodans* carries a mixture of *p*-hydroquinone and hydrogen peroxide. This mixture is metastable, i.e., the two components do not react with each other in the absence of an external stimulus. When the bombardier beetle feels itself to be endangered it adds two catalysts, an oxidase and a catalase, from its glandular system. Hydroquinone is then oxidized explosively according to equation (1) while the loud noise of the steam emitted frightens the natural enemy away. Catalysis chemistry as survival strategy – in nature!



This defense reaction of the bombardier beetle demonstrates another aspect of the nature of catalysis. Catalytic processes must be thermodynamically allowed. *Allowed* reactions become *spontaneous* reactions when the initially high barrier to reaction is lowered by a catalyst. A selective catalyst is additionally characterized by the fact that it only opens up one of several possible reaction pathways. This means that a selective catalyst kinetically favors “its reaction” over the other feasible possibilities. Thus catalysts discriminate also by way of the reaction rates.

Although aimed at a general understanding, the above description already gives an idea of the enormous potential of catalysis. Practically all chemical reactions, provided that they are indeed thermodynamically allowed, can be realized with the help of suitable catalysts. The wide variety of the material world still lies in front of us, not behind us. On the other hand, the search for specific, efficient catalysts becomes more and more difficult the higher our expectations with regard to the activity, the specificity, and the lifetime of a catalyst are. From an economic point of view a catalyst may be expensive and have a short lifetime when it enables the production of a correspondingly high-value product. The ecological advantage is then largest when the use of a catalyst avoids the formation of by-products that are highly toxic or that have no use in other process cycles. Of course, from an ecological point of view, catalysts that achieve the chemical disposal of mass products are particularly sought after; these include numerous organic plastics, above all, polyethylene, polypropylene, and polyvinyl chloride (PVC).

From Catalytic Table Lighter to Technical Catalysis

The word catalysis originates from the Greek $\kappa\alpha\tau\alpha\lambda\epsilon\iota\nu$ and means as much as *to untie* or *to pick up*. The term was introduced by *Berzelius* (1835) while *Döbereiner*

spoke of “contact action” and *Mitscherlich* (1831) referred to “contact processes”. In 1823 *Döbereiner* discovered the catalytic action of the noble metal platinum on a mixture of hydrogen and oxygen. The lighter named after him turned out to be an enormous success. It is estimated that in the 1820’s over one million examples in various shapes and sizes were sold: fire without tinder and flint, an achievement of catalysis! Today, this, the simplest of all chemical reactions, is a major topic in the development of alternatives to the internal combustion engine for vehicle propulsion.

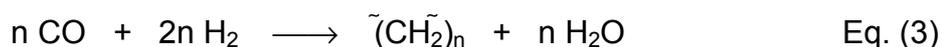
Progression from the catalytic table lighter to industrial-scale catalysis required one hundred years. Again hydrogen was involved but its reaction with elemental nitrogen was much more difficult than that with oxygen. The exothermic ammonia synthesis from the elements according to equation (2) was realized by *Haber, Mittasch and Bosch* with the help of heterogeneous catalysts. While the first technical reactors (1913) required 300 kg of an iron-based catalyst to produce 5 tons of ammonia per day, a modern reactor yields about 1500 tons per day. The specific energy needs decreased from around 90 GJ per ton of ammonia in 1950 to today’s value of just a little above the theoretical amount (20 GJ). When today more than 100,000,000 tons of ammonia per year are produced by the original process, it must be remembered that the Haber-Bosch process was a blessing for mankind at that time. The inability to feed a rapidly growing population predicted by Malthus in his “Essay on Population” (1798) did not become reality only because *Carl von Linde* (1897) had taught us how to liquefy the air and because *Fritz Haber* had succeeded in producing ammonia catalytically from the thus enriched nitrogen as the basis for nitrogen fertilizers. Without a catalyst the elements nitrogen and hydrogen react so slowly that we would today still be waiting for the first gram of ammonia.



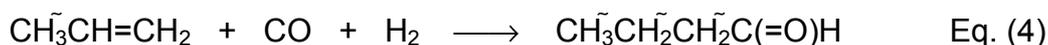
In the mean time we know rather precisely what activation steps occur at the catalyst surface. Only very few surface atoms are really active: so-called step and kink domains at which di- or polyatomic molecules are absorbed, initially physically then chemically, and are subsequently cleaved into active atoms or fragments. Today, highly developed analytical methods are available to study the physics and chemistry of surfaces in order to examine the elemental steps of catalysis – at least on a reality-

near model. In contrast, it is still difficult under real conditions – usually high pressure and high temperature – to directly observe the microscopic reaction process. Research on this aspect is urgently needed.

The domain of organic raw materials was opened up when *Franz Fischer* and *Hans Tropsch* in the Mulheim Kaiser Wilhelm Institute (from about 1920) found out how to hydrate the then technically available carbon monoxide [Equation (3)]. Once again exothermic, this reaction produced for the first time higher molecular products among which the liquid hydrocarbons would later gain importance as “synthetic petrol”. The *Fischer-Tropsch* process suffers from a low selectivity. In the present age of crude oil it is only economically relevant in regions where coal is extremely cheap and oil extremely expensive. The plant operating with German technology (LURGI) in Sasolburg, South Africa, is the largest in the world for this form of coal processing. A plausible model has been proposed for the mechanism of this catalytic process.



Consequent research work on the optimization of *Fischer-Tropsch* catalysts opened up a completely new field, namely that of *homogeneous catalysis*. This operates with molecular catalysts which, on account of their clear and defined structures, permit a much better understanding of their modes of action than any solid catalyst. And, one catalyst molecule behaves in exactly the same way as the next. When *Otto Roelen* at Ruhrchemie, Oberhausen observed the formation of butyraldehyde from ethylene, carbon monoxide, and water [Eq. (4)] in 1938 he could not have guessed that this reaction would be the prototype for an organometallic homogeneous catalysis that has reached a yearly capacity of ca. 9,000,000 tons of product in the year 2000. At that time the catalyst was hydridotetracarbonylcobalt, $\text{HCo}(\text{CO})_4$, while today the much more reactive and selective phosphane complexes of rhodium are used technically. Systematic catalyst development has resulted in modern processes requiring 30 ppm rhodium loading, with the costs for the catalyst ligand being higher than those for the (noble) metal of the catalyst. Even as little as ten years ago the most optimistic expert would not have dared to make such predictions.



Organometallic Catalysis

The time only became ripe for the large-scale technical homogeneous catalysis with the dramatic development of organometallic chemistry during the 1950's and 1960's. This new chemistry of the transition metals with its apparently inexhaustible variations in bonding and coordination appeared to provide an ideal starting point for finely tuned, tailored catalysts. Individual examples of scientific and economic brilliance have had an almost magic effect on technical catalysis: *Ziegler* and *Natta's* olefin polymerization (1954/1955) with a current production volume of at least 75,000,000 tons per year, the acetaldehyde process from Wacker Chemie GmbH (1959), and the Monsanto acetic acid process (1970) with today a world capacity of around 2,500,000 tons per year. However, the developments are not only reflected by the large amounts, the recognition that chiral catalyst ligands – initially verified with a series of organophosphanes – could effect optical induction on prochiral substrates was also a major breakthrough. Stereoselective synthesis with the help of organometallic catalysts was thus born and the anti-Parkinsonian drug L-DOPA was the first technical example in the field of pharmacy. Chiral information can be multiplied hundreds or even thousands of times. Chirality transfer is the most valuable type of catalysis and is now indispensable for modern pharmaceutical chemistry with its high demands on quality.

Although the older catalytic processes, especially those less stereoselective examples of heterogeneous catalysis, have been further optimized, the new organometallic chemistry of the 1970's and 1980's has led to classes of substances fulfilling ever increasing demands. In some such cases the structural principles of long-known reactions have been appeared again: thus, E. O. Fischer's metal-carbene complexes induce olefin metathesis reactions that now constitute an exciting development in industrial practice. The so-called stereo-rigid metallocene derivatives represent an unexpected highlight. As a consequence of their constrained conformational situation, this class of compounds has been developed in fifteen years of intensive research to the most brilliant of all known catalytic systems. Thus, it is today possible by means of relatively small structural changes on a basic substance to produce a large variety of literally tailored molecular catalysts, i.e.,

catalysts that are exactly constructed for a specific purpose. With their help a palette of homo- and copolymeric products from the olefin series has recently become available. These include not only a highly isotactic polypropylene on a zirconocene base but also copolymerizates for compact disc materials. Enzyme-like activities of over 1 ton product per gram of catalyst metal and hour – at merely 60 °C – are typical, this corresponds to a TOF of more than 2,500,000 per hour. Unfortunately at the time when the metallocene catalysts were discovered by *Brintzinger* and *Kaminsky* in 1985 the methods of theoretical chemistry were not sufficiently developed for an optimization by mathematical simulation of these relatively electron-poor systems. Things have changed since then, density function calculations in combination with molecular mechanics considerations and today's high performance computers now allow trends to be predicted with adequate reliability.

A convincing example for the performance of chiral organometallic catalysts is provided by the menthol synthesis of the Takasago Pharmacy Co. Ltd. About half of the market for natural (laevorotatory) menthol is now produced from the cheap myrcene, C₁₀H₁₆, in 7-ton batch reactors. The key step is the highly stereoselective rearrangement of an allylamine to the corresponding ynamine. The first stereocenter is constructed in almost 100% selectivity with the help of a rhodium-BINAP catalyst; this is followed by the classical sequence of hydrolysis, ring closure, and hydration. Thus, in addition to high-priced pharmaceutical products, the less expensive fine chemicals field also benefits from molecular catalysis. The current status, performance, and perspectives of organometallic, homogeneous catalysis are described in detail in a two-volume work³⁾ and hence further examples will not be mentioned here.

Catalysis: Current Challenges

Experts agree that catalysis is a high technology of all-encompassing value. The production of many raw and fine chemicals as well as pharmaceutical products is only possible by means of catalytic processes, either to avoid undesired, interfering, or hazardous by-products (especially with bulk chemicals) or as an indispensable step in the case of specific stereochemical synthesis requirements for pharmaceutical agents. One can, in fact, safely prophesy that specifically active catalysts will be the

only way to degrade plastics after they have served their purpose. First examples for the degradation of polyethylene and polypropylene were recently presented⁸; However, these processes cannot (yet) tolerate the contaminants usually accompany used plastics and mixed polymerizates.

Besides the materials field through to *life science* products, *energy research* would also not make much progress without catalysis. The storage of energy, perhaps the major topic in energy research, is based on catalytic processes, irrespective of whether we consider the chemical processes occurring in batteries or hydrogen technology. A fuel cell is usually preceded by the chemical conversion of “stored energy”, i.e., a catalytic reforming process (e.g., methanol/water) with its sensitive dependence on pressure, temperature, and technical system. The demands for *robustness* and *efficacy* for such reforming catalysts are extremely high in the light of the expectation that within 20 years the proportion of fuel-cell driven vehicles will amount to about 20%, i.e., 10,000,000 private motor vehicles in Germany. The safety problems associated with a vehicle fuel tank containing hydrogen under pressure will only be eliminated when an alternative fuel such as methanol can be efficiently converted by a catalytic process into a gas with high hydrogen content immediately prior to combustion.

We can expect that catalysis for vehicle propulsion will achieve a similar success as that for cleaning vehicle exhaust gases. The 3-way catalytic converter for the three pollutant groups nitrogen oxides, carbon monoxide, and hydrocarbons operates on a noble metal base (platinum, palladium, rhodium). In spite of its good performance, this is still an “*end of the pipe*” solution. Even so, the engines of motor vehicles remain the most abundant “chemical reactor” in the world (about 1 billion in number). They depend on gasoline, the sulfur and aromatic contents of which must again be drastically reduced to comply with EU regulations. Considering the round 180,000,000 tons per year of gasoline consumed in Europe this represents an enormous challenge for catalyst technology, the only possibility to solve the problem.

High expectations are being set on light-driven catalysts, the so-called *photocatalysts*. Their principle of action involves a catalyst, applied as a thin film on a supporting surface, that generates two active sites under the action of light, namely

positively charged defects and free electrons. These two species undergo differing chemical reactions, especially redox reactions. One such photocatalyst is semi-conducting titanium dioxide⁹. It generates hydroxy radicals ($\cdot\text{OH}$) and superoxide ions (O_2^-) from water and oxygen by oxidation and reduction, respectively. Photocatalysts are already in commercial use for the generation of antibacterial and antiviral properties, for purifying circulating air or water, and in cancer therapy. The potential for development of photocatalysts cannot yet be foreseen and is mainly unexplored.

Just as important as the catalysts themselves are the corresponding process technologies^{10, 11}). This is mainly a task for the engineer. There is a difference whether the catalyst is soluble in the reaction medium or not, whether it has a defined molecular structure or is a solid, whether it is volatile or not, stable in air or pyrophoric. The process technology also depends on whether the catalyst is used as a pure substance or is fixed on a support. Finally, it is relevant whether the reaction proceeds in the homogeneous phase or in a two- or multi-phase system and whether it is mainly thermoneutral or highly exothermic. The process technology addresses all of these conditions encompassing the entire spectrum of catalytic procedures. The process may be operated in a continuous or a non-continuous (batch) mode. Exploitation of the heat of the reaction is of economic importance and this frequently has a major influence on the design of the plant. Even when homogeneous catalysts are often active at room temperature on account of their defined and reproducible structures, process temperatures of above 100 °C (e.g., 140 °C for two-phase hydroformylation) are usually selected in order to use the reaction heat in the plant itself or a combination of plants, e.g., for distillative product purification. Thus catalysis research includes the entire field from the chemistry of molecular catalysts and solid reactions to plant engineering and process control. Miniature flow-through cells are a step on the way to the development of catalytic bioreactors.

Catalysis: An Attempt at Evaluation

Catalysis is the tool to perform chemical reactions in a specific manner with the least possible consumption of substances and energy. In view of the enormous number of material transformations and the associated feedstock, energy, and waste problems,

catalysis is *the scientific topic* with the highest priority. It is a prerequisite not only for growth but also for the management of a world depending on a differentiated spectrum of materials. Thus, catalysis is simultaneously also an *ecological, economic, and political* topic. That politicians have not yet recognized these relationships is surprising even when the increasing shortages of energy and raw materials are not taken into consideration.

The Scientific Dimension

Chemical products are attractive when they display advantageous properties. This is true not only for the insulating, air-permeable artificial fibers but also for anti-cancer drugs. The properties of the product are related to its chemical structure and the preparation of the substance is oriented to its structure. Many production processes have the disadvantage that they must either use inappropriate starting materials or that they also produce unwanted by-products. A common reason for this is that the specific construction from simple precursors does not work because the reaction route has a high activation barrier and that the catalysts necessary to lower this barrier are not available. There is a need here for much more research. It is found again and again that applied research, that is research on a specific object, on the basis of sound basic research is necessary. The thousands and thousands of old as well as new products will require an enormous expenditure in research. However, the benefits from just this research will certainly be of immense value. The testing of numerous catalyst variations which seemed hopeless in terms of effort is now slowly acquiring a firm foundation. The advances in miniaturization and automatic techniques (microsystem techniques) have resulted in processes by which a parallelized catalyst development is possible. Many different catalysts are handled by an automatic sampling system so that now an accelerated, combinatorial catalyst screening has become reality¹²⁾. This development, as is used, for example, by Symyx Corp (Palo Alto, CA) for organometallic homogeneous catalysts, is currently revolutionizing classical catalysis research. Germany will have a special chance in this field if highly advanced scientific cultures, synthetic chemistry on the one hand and microsystem techniques and robotics on the other hand, can be made to work hand in hand. This demonstrates that a further compartmentalization of the natural

and engineering sciences will be detrimental to a field of technology with the potential to revolutionize the world of tomorrow.

A second major chance for catalysis is opened up by the fact that modern super computers can handle model calculations. The programs for these calculations, developed in the past years by trial and error methods will not become obsolete but will be supplemented by highly sophisticated model calculations able to closely approach complicated molecular structures. Sound laboratory chemistry based on computer-assisted model considerations and parallelized catalyst screening through miniaturized process technology will be the recipe for success in the new “combinatory catalysis chemistry”. Catalysis on the nanogram scale will place new demands on chemistry. Thus, the question is posed as to how such small amounts of substance will behave on passage through miniaturized reaction channels – a challenge for catalyst chemistry!

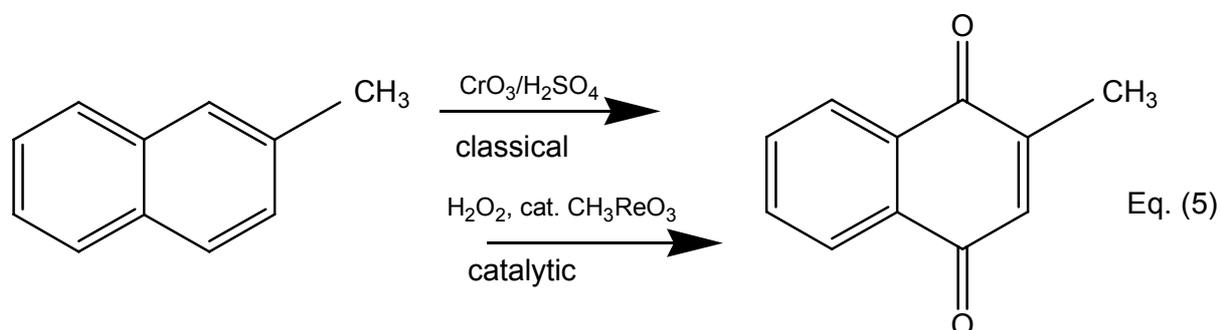
The Ecological Dimension

Durability is a principle to which chemistry is duty bound in a special way. Each and every change in a material involves the chemistry of the material and is, therefore, a chemical process. Our work as chemists is effective when we reduce the waste or toxic by-products of a chemical synthesis by choosing alternative synthetic routes starting, whenever possible, from simple and cheap raw materials. The search for efficient catalysts plays a major role in this process since “slender reaction routes” are not realizable in any other way¹⁾.*

An example worthy of mention is the new synthesis according to equation (5) of vitamin K₃, which is used ubiquitously in veterinary medicine in the USA and is important as an anticoagulation vitamin for newborn babies in human medicine. Classically, vitamin K₃ is produced by the oxidation of 2-methylnaphthalene using chromic acid. This furnishes 16 kg of toxic, chromium-containing waste per kg of

* Under this term the author means a reaction step or sequence with the best possible economic total balance in terms of atoms. This again implies that as many atomic components as possible of the starting materials occur in the product and are thus fully exploited. If this is not possible on account of the composition of the product, then only ecologically harmless by-products (inevitable accumulation) should be formed in a slender reaction, for example, water or easily separable gases (CO, CO₂).

product. The new catalytic route uses hydrogen peroxide in combination with the very efficient homogeneous catalyst methyl(trioxo)rhenium, CH_3ReO_3 ^{14a)}.



The same catalyst also enables the oxidative preparation of vanillin from biowastes^{14b)} and the oxidation of starches^{14c)}, in both cases in combination with the cheap, environmentally harmless oxidizing agent hydrogen peroxide.

The ecological dimension is even clearer when the shortage of the fossil chemical raw materials, crude oil and coal, is taken into consideration. Since we can no longer do without the highly differentiated product palette derived from coal and crude oil, alternative approaches are urgently needed. Natural gas may offer a temporary alternative if its CH-activation by catalytic means can be realized. For the long-term, however, I consider regenerable raw materials to be the only feasible solution.

Even so, we must first assure that plants can grow rapidly~ also on soils that are not always rich in nutrients~ and produce specific component substances that make harvesting worthwhile, This objective cannot be reached chemically and economically without the help of plant genetics; this, however, is a separate topic. In any case, only the catalytic further processing of such component compounds will ultimately replace those products based on coal and crude oil. Regenerable raw materials will thus take over from the product spectra of classical chemistry; this means that we will be starting from a higher, i.e., more complex material level. This vision will remain a vision without the help of catalysis research.

Catalysis is also the method of choice for avoiding pollutants irrespective of whether they are of natural or man-made origin. The large-scale example of motor vehicle exhaust gas catalysts is an adequate illustration and the use of fuel cell technology

for the primary objective of reducing vehicle emissions has been mentioned above. All major automobile concerns are active in this field. Selective, efficient, and long-lasting catalysts are the key to success. It has just recently been reported in *Nature* that the use of natural gas as a fuel is possible with the help of copper and samarium oxide-containing catalysts¹⁵⁾.

The Economic Dimension

A few years ago, the "Board of Chemical Sciences and Technology" reported to the President of the USA that catalysis has the significance of a national, key technology: *"Our current position of world leadership can be attributed to our strength in the field of chemical catalysis."* It is estimated that 20% of the gross national product of the USA *"is generated through the use of catalytic processes that assist in satisfying such diverse societal needs as food production, energy conservation, defense technologies, environment protection, and health care. On the horizon, the extensive use of catalysis will tap new energy sources... Chemical catalysis will figure strongly in the health of our chemical industry... Organometallic catalysis will continue as a large active branch of chemistry involving synthesis"*.¹⁶⁾

In fact, the market for catalysts amounts to ca. 12 billion US \$ per year with an estimated product market of 1.2 – 6 quadrillion US \$ (factor of 100 – 500). Thus, > 80% of the net product of the chemical industry alone is based on catalytic processes¹⁷⁾. With ca. 4%, Germany occupies an insignificant position among the manufacturer's of catalysts, a dubious situation for a developed country.

The strategic position of catalysis among the future technologies is even more far-reaching for Germany and Central Europe as our geopolitical importance is becoming increasingly strongly linked to technical innovations that can easily be exported and are in the upper regions of the net product chain. A new catalyst is practically always associated with a new product, a new procedure, or a new service. Catalysts are always coupled with material transformations and material transformations are the task of the chemical industry including the *life sciences*. Just in the latter field, that of medicine and health, there is practically unlimited growth potential. New catalysts are

literally job-producing machines since they enable further differentiation in the chemical industry and all its associated branches (e.g., pharmaceuticals).

A recent success story is that of the already mentioned metallocenes that were developed to market maturity in competition between Dow Chemical and Exxon on the one hand and Hoechst and BASF on the other hand. The German activities are now combined in the joint-venture company TARGOR. In the R&D phase, decisive advances originated from just a few German university laboratories with essential competence in organometallic catalysis; process technological problems were solved by the industry. This example shows that every catalyst can be developed from a laboratory curiosity to a technical product when the economic prospects seem to justify the expenditure of effort.

Prosperous companies or individual branches of the chemical and pharmaceutical industries often owe their success to a specific catalyst know how. Thus, the new two-phase process for hydroformylation developed by the former Ruhrchemie AG (since 1984, now Celanese) has been licensed worldwide. At the same time it represented a breakthrough that combined the advantages of homogeneous and heterogeneous catalysis. In oxidation catalysis, probably the most important refinement sector, most problems have not been solved because there are hardly any selective oxidation catalysts for sufficiently cheap, ecologically harmless oxidation processes. Even so, chemists of the Italian Enichem have been able since 1990 to convert the chemical feedstock propylene into the versatile intermediate propylene oxide. The key to success of this million ton product is the so-called titanium silicate catalyst TS-1. It belongs to the class of the zeolites, mineral materials with special cavity and channel structures. Enichem's trick for this new type of solid catalyst involves the specific positioning of "foreign" titanium atoms in strategically important lattice positions. However, this remains an excellent but isolated example.

For many other products, success depends on the catalyst and application know how. This is the reason why, for example, Vinnolit GmbH in Gendorf (formed by a combination of branches of Hoechst and Wacker) does not use its process for ethylene chlorination alone but has granted worldwide licenses. Shell is in a similar position with a series of catalytic processes including ethylene oxidation

(silver/rhenium/cesium catalysts) and, more recently, an elegant process for the production of polyketone plastics for automobile parts (palladium chelate catalysts). The inventor of a new catalyst is in an unrivaled position because patent protection for a catalyst implies its use for the preparation of old and new products. And this is the important point. Catalysts are door-openers, however, the codes to open the locks are difficult to obtain. It is also true for chemical products that although many roads lead to Rome, the one with the least obstacles wins.

The Political Dimension

The scientific, ecological, and economic evaluations converge to a *political topic*. Politicians do not discover new catalysts but they do create the conditions required by talented researchers. In Germany there are many “split valences” but on the whole catalysis research does not have its own shape. It does not exhibit an international profile in spite of the individual major successes in the motherland of catalysis.

There is a need for research policies at regional and national government levels in the sense of a national program. Starting from the regional “hot spots” at which catalysis research is beginning to consolidate in spite of its variety, a national organization should be founded to exert a potentiating and solidifying influence on the available competence. This is the only way to develop the future technology catalysis. In Bavaria, there is a research union (FORKAT) that combines university and industrial research efforts. A catalysis union according to this example is being created in North Rhine-Westphalia. This marks out a way to make the new generation of researchers aware of catalysis. However, regional charters are not enough, we need a united national solution with a visible headquarters.

Other countries have recognized the chances of united efforts without giving up their wealth of inventiveness and just for these reasons need a targeted “applied research”. For example, Holland has initiated a consequent research network for catalysis (NIOK) and has thus brought the best research groups from university and industry together. Even Spain and Portugal, previously not serious contenders in the fields of chemical and pharmaceutical research, are successfully catching up; new research centers are being built and manned by people from all over the world. China

is sending its talented researchers to catalysis laboratories in Germany. Then China has also realized that highly refined products are indispensable for success on the world market. After 200 years of humiliation¹⁸⁾ the country is rearming with the help of high technologies. It is interesting, and at the same time tragic, that the country with the oldest civilized culture foundered from about 1800 because of the lack of technical modernization demanded by a rapidly expanding population. The analogous problem in Europe was solved by technical advances, among others, in chemical products such as, e.g., ammonia as fertilizer. The recipe for success was catalysis.

In spite of the encouraging successes of German companies in the C&I technologies the economy will continue to depend on a strong and innovative chemical and pharmaceutical industry. Even with all its turbulences, the German chemical industry has a domestic turnover of ca. DM 190 billion and a foreign turnover of DM 100 billion and still belongs among the largest in the world. With the fusion of Degussa/Hüls/SKW the world wide largest special chemical concern (initial turnover ca. DM 34 billion) has been created in Germany. This will depend to a major extent on catalytic production processes on the one hand to achieve the necessary product palette and on the other hand to establish itself in new constellations with regard to feedstock and intermediate products.

Thus, it is clear that, besides the nation as upholder and sponsor of the research community, the industry as its major beneficiary must also take part in the major task of catalysis research. The nation must support young talents and provide them with the best possible educational possibilities at home and abroad while the industry should accompany, shape, and help finance the research work of these talented young people.

Germany could rapidly become the leading nation in catalysis research and applications when it declares itself to the topic and takes the necessary action. In contrast to the "green gene technology" which Germany, unlike the USA and China, has more or less given up, we do not have to apply for acceptance of catalysis technology, it is already there. So, what are we waiting for?

Key References and Suggestions for Further Reading

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