ANGEWANDTE CHEMIE

Volume 27 · Number 12
December 1988
Pages 1593–1764

International Edition in English

Under the Surface of the Chemical Article**

By Roald Hoffmann*

You open an issue of a modern chemical periodical, say the important German *Angewandte Chemie*[1] or the *Journal of the American Chemical Society,* and what do you see? Riches upon riches: reports of new discoveries, marvelous molecules, unmakeable, unthinkable yesterday—made today, reproducibly, with ease. The chemist reads of the incredible properties of novel high-temperature superconductors, organic ferromagnets, and supercritical solvents. New techniques of measurement, quickly equipped with acronyms—EXAFS, INEPT, COCONOESY—allow you to puzzle out the structure of what you make more expeditiously. Information just *flows.* No matter if it's in German, if it's in English. It's chemistry—communicated, exciting, alive.

Let's, however, take another perspective. To the pages of the same journal turns a humanist, a perceptive, intelligent observer who has grappled with *Shakespeare, Pushkin, Joyce,* and *Paul Celan.* I have in mind a person who is interested in what is being written, and also in how and why it is written. My observer notes in the journal short articles, a page to ten pages in length. She notes an abundance of references, trappings familiar to literary scholars, but perhaps in greater density (number of references per line text) than in scholarly texts in the humanities. She sees a large proportion of the printed page devoted to drawings. Often these seem to be pictures of molecules, yet they are curiously iconic, lacking complete atom designations. The chemist's representations are not isometric projections, nor real perspective drawings, yet they are partially three-dimensional.

My curious observer reads the text, perhaps defocusing from the jargon, perhaps penetrating it with the help of a chemist friend. She notes a ritual form. The first sentences often begin: "The structure, bonding and spectroscopy of molecules of type X have been subjects of intense interest.[a–z]" There is general use of the third person and a passive voice. She finds few overtly expressed personal motivations, and few accounts of historical development. Here and there in the neutered language she glimpses stated claims of achievement or priority—"a novel metabolite", "the first synthesis", "a general strategy", "parameter-free calculations". On studying many papers she finds a mind-deadening similarity. Nevertheless, easy to spot in some of the articles, she also sees style—a distinctive, connected scientific/written/graphic way of looking at the chemical universe.

I want to take a look, now not hiding behind this observer, at the language of my science, as it is expressed in the essential written record, the chemical journal article. I will argue that much more goes on in that article than one imagines at first sight; that what goes on is a kind of dialectical struggle between what a chemist imagines should be said (the paradigm, the normative) and what he or she must say to convince others of his or her argument or achievement. That struggle endows the most innocent-looking article with a lot of suppressed tension. To reveal that tension, I will claim, is not at all a sign of weakness or

[*] Prof. R. Hoffmann
Department of Chemistry, Cornell University
Ithaca, NY 14853 (USA)

[**] This article is derived from the text of a lecture I presented at the Chemiedozententagung in Mainz on March 14, 1988. At a special session of that meeting the 100th anniversary of *Angewandte Chemie* was celebrated.

irrationality, but a recognition of the deep humanity of the creative act in science.

The Scientific Article: A Brief History

There was chemistry before the chemical journal. It was described in books, in pamphlets or broadsides, in letters to secretaries of scientific societies. These societies, for instance the Royal Society in London, chartered in 1662, played a critical role in the dissemination of scientific knowledge. Periodicals published by these societies helped to develop the particular combination of careful measurement and mathematization that shaped the successful new science of the time.[2]

The scientific articles of the period are a curious mixture of personal observation and discussion, with motivation, method, and history often given firsthand. Polemics abound. Cogent arguments for the beginning of a codification of the style of the scientific article in France and England in the 17th century have been given by *Shapin*,[3a] *Dear*,[3b] and *Holmes*.[3c] I think the form of the chemical article rigidified finally in the 1830s and 1840s and that Germany was the scene of the hardening. The formative struggle was between the founders of modern German chemistry—people such as *Justus von Liebig*—and the *Naturphilosophen*. In that particular period the latter group might be represented by *Goethe*'s followers, but their like was present elsewhere in Europe even earlier, in the eighteenth century. The Natural Philosophers had well-formed notions, all-embracing theories, of how Nature should behave, but did not deign to get their hands dirty to find out what Nature actually did. Or they tried to fit Nature to their peculiar philosophical or poetic framework, not caring about what our senses and their extension, our instruments, said. The early 19th century scientific article evolved to counter the pernicious influence of the Natural Philosophers. The ideal report of scientific investigation should deal with the facts (often labeled explicitly or implicitly as truth; more on this later). The facts had to be believable independent of the identity of the person presenting them. It followed that they should be presented unemotionally (so in the third person) and with no prejudgment of structure or causality (therefore the agentless or passive voice).

The fruits of this model reportage were immense. An emphasis on experimental facts stressed the reproducible.

1176

211. Fr. Goldmann: Ueber Derivate des Anthranols.

(Vorgetragen vom Hrn. Professor Liebermann.)

In einer früheren Mittheilung¹) habe ich über die Einwirkung von Brom auf Anthranol berichtet und ein dabei entstehendes Dibromsubstitutionsproduct als analog dem Anthrachinondichlorid von Thörner und Zincke bezeichnet. Die Bildung des Anthrachinondichlorides war hiernach bei der Einwirkung von Chlor auf Anthranol zu erwarten.

Anthrachinondichlorid, Dichloranthron, $C_6H_4 \left\langle {}^{CO}_{CCl_2} \right\rangle C_6H_4$

In eine kalte concentrirte Lösung von Anthranol in Chloroform wurde während etwa 20 Minuten trockenes Chlorgas geleitet, wobei die Lösung auf Zimmertemperatur erhalten wurde. Nach beendeter Reaction, bei der reichliche Chlorwasserstoffentwicklung stattfand, wurde das Chloroform auf dem Wasserbade verjagt, der Rückstand mit heissem Ligroïn ausgezogen und das in Lösung gegangene Product aus einer heissen Mischung von Benzol und Ligroïn umkrystallisirt.

Die Substanz wird so in Form von wasserklaren dünnen Prismen erhalten. Dieselben schmelzen bei 132–134°.

Die Verbindung ist in Benzol, Schwefelkohlenstoff, Chloroform sehr leicht, in kaltem Ligroïn oder Aether ziemlich schwer löslich. Aus der Schwefelkohlenstofflösung erhält man die Substanz beim Verdunsten in schönen wasserklaren Krystallen.

	Gefunden		Ber. für $C_{14}H_8OCl_2$
C	64.62	—	64.12 pCt.
H	3.25	—	3.05 »
Cl	—	26.96	26.72 »

Durch Kochen mit Eisessig oder Alkohol wird die Verbindung vollständig in Anthrachinon übergeführt. Die Chloratome müssen daher in der Mittelkohlenstoffgruppe sich befinden. Die Verbindung ist hiernach und nach ihren Eigenschaften mit dem Anthrachinondichlorid, welches Thörner und Zincke²) bei der Einwirkung von Chlor auf *o*-Tolylphenylketon erhielten, indentisch.

¹) Diese Berichte XX, 2436.
²) Diese Berichte X, 1480.

1177

Aus dem Anthranol entsteht sie nach der Gleichung:

$$C_6H_4 \left\langle {}^{C(OH)}_{CH} \right\rangle C_6H_4 + 2Cl_2 = C_6H_4 \left\langle {}^{CO}_{CCl_2} \right\rangle C_6H_4 + 2HCl.$$

Hr. Privatdozent Dr. A. Fock hatte die Güte, mir über die Krystallform des aus Schwefelkohlenstoff auskrystallisirten Anthrachinondichlorides Folgendes mitzutheilen:

Die Krystalle sind monosymmetrisch:

$$a : b : c = 0.7973 : 1 : 0.6262.$$
$$\beta = 72^\circ 48'.$$

Beobachtete Formen:

$$m = \infty P(110),\ c = oP(001),\ p = -P(111).$$

Die Krystalle bilden schwach gelblich gefärbte dünne Prismen, die Basis tritt nur an einzelnen Individuen und zwar ganz untergeordnet auf.

		Beob.	Berechnet
m : m	= 110 : 1̄10	= 74° 36′	—
m : c	= 110 : 001	= 76° 24′	—
p : c	= 111 : 001	= 37° 54′	—
p : p	= 111 : 11̄1	= 45° 30′	45° 2′
p : m	= 111 : 110	= 38° 38′	38° 30′
p : m	= 111 : 1̄10	= —	71° 25′

Spaltbarkeit nicht beobachtet.

Auch das analoge Anthrachinondibromid hat Hr. Dr. Fock zu messen die Güte gehabt, wobei er folgende Resultate erhielt:

Die Krystalle sind monosymmetrisch:

$$a : b : c = 1.5009 : 1 : 1{,}4708.$$
$$\beta = 70^\circ 43'.$$

Beobachtete Formen:

$$c = oP(001),\ p = -P(111),\ o = +P(\bar{1}11),$$
$$q = \tfrac{1}{2} P \infty (012),\ w = +2P2(\bar{1}21).$$

Schwach gelblich gefärbte Krystalle von 1—4 mm Grösse und recht verschiedenartiger Ausbildung. Meistens herrschen die Flächen der vorderen Pyramide p und der Basis vor, während die übrigen nur ganz untergeordnet ausgebildet sind. Bisweilen sind die Flächen der Pyramide w grösser ausgebildet und zwar theilweise nur einseitig, so dass die Krystalle eine ganz verzerrte Ausbildung erhalten.

Fig. 1. The first two pages of a typical article from 1888 [4].

The conciseness of the German language seemed ideally suited to the developing paradigm. Cadres of chemists were trained. The development of the dyestuff industry that followed in England and Germany is a particularly well studied manifestation of the industrial application of the new, organized chemistry.

The scientific article acquired in this period a canonical or ritual form. In Figure 1, I reproduce part of a typical article of that period.[4,5] Note most of the features of a modern article—references, experimental part, discussion, diagrams. All that's lacking is the acknowledgment thanking the Deutsche Forschungsgemeinschaft or the National Science Foundation.

In Figure 2, a contemporary article, we approach the present. This particular contribution, an important one by *O. J. Scherer* and *T. Brück*[6] reports a remarkable ferrocene-type system in which one cyclopentadienyl ring has been replaced by P_5. The work is novel and significant, but I want to focus on the mode of presentation rather than the content. How does this article differ from one published a hundred years ago? The dominant language has changed, for interesting geopolitical reasons, to English.[7] Yet it seems to me that there is not much change in the construction or tone of the chemical article. Oh, marvelous, totally new things are reported. Measurements that took a lifetime are made in a millisecond. Molecules unthinkable a cen-

$[(\eta^5\text{-}P_5)Fe(\eta^5\text{-}C_5Me_5)]$, a Pentaphosphaferrocene Derivative**

By *Otto J. Scherer** and *Thomas Brück*

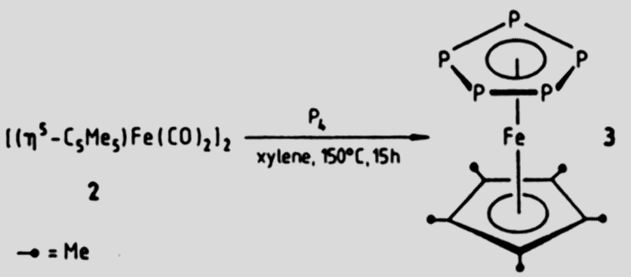
After having demonstrated that *cyclo*-P_5 could be stabilized as bridging ligand in the mixed-valence triple-decker complex **1**,[1] we then attempted to realize the classical

$[(\eta^5\text{-}C_5Me_5)Cr(\mu,\eta^5\text{-}P_5)Cr(\eta^5\text{-}C_5Me_5)]$

1

sandwich coordination of this ligand (cyclo-$P_5^{\ominus}$ as 6π electron donor). Success was achieved upon cothermolysis of **2** with white phosphorus.

Pentamethylpentaphosphaferrocene **3** forms sublimable, green crystals which can be handled in the presence of air and which begin to melt (with partial sublimation and slight decomposition) at 270°C when heated in a sealed tube. **3** is very soluble in dichloromethane, readily soluble in benzene and toluene, and moderately soluble in pentane.



In the ^{1}H-NMR spectrum (200 MHz, 293 K, C_6D_6, TMS int.) of **3** a sharp singlet is observed at $\delta = 1.08$ which is shifted 0.6 ppm upfield compared to that of decamethylferrocene $[(\eta^5\text{-}C_5Me_5)_2Fe]$ **4**.[3] In comparison to the $^{13}C\{^1H\}$-NMR signals of **4**,[2,3] those of **3**[2] are shifted slightly downfield. The $^{31}P\{^1H\}$-NMR signal shows a continuous downfield shift within the series triple-decker **1** ($\delta = -290.5$[1]), monophosphaferrocene $[(\eta^5\text{-}C_5H_5)Fe(\eta^5\text{-}PC_4H_4)]$ **5** ($\delta = -67.5$[4]), **3** (81.01 MHz, C_6D_6, 85% H_3PO_4 ext., $\delta = 153.0$ (s)), and $Li(P_5)$ ($\delta = 470$[5]). In the mass spectrum,[2] the most intense peak is the molecular peak of **3**, followed by the peak for $M^{\oplus} - P_2$. So far, all attempts to prepare a single crystal suitable enough for an X-ray structure analysis have failed, both by sublimation as well as recrystallization. *cyclo*-$P_5^{\ominus}$ is probably formed from $P_3^{\ominus}$ and P_2.[6]

[*] Prof. Dr. O. J. Scherer, Dipl.-Chem. T. Brück
Fachbereich Chemie der Universität
Erwin-Schrödinger-Strasse, D-6750 Kaiserslautern (FRG)

[**] This work was supported by the Fonds der Chemischen Industrie.

Experimental

A mixture of **2** [7] (980 mg, 2.3 mmol) and P_4 (1500 mg, 12.1 mmol) in xylene (80 mL) was stirred under reflux for 15 h and the insoluble material removed by filtration on a D3 frit and extracted three times with 80 mL each of CH_2Cl_2 (393 mg of residue after drying under high vacuum). The solvent was removed from the combined extracts under oil-pump vacuum. After three extractions with 50 mL each of pentane there remained 726 mg of a brown solid whose composition could not be unequivocally established. After removal of the solvent from the green extracts (oil-pump vacuum), the residue remaining behind was sublimed. At 60°C/0.01 torr, excess phosphorus was removed; between 90° and 110°C, green needles sublimed on the wall of the glass vessel. Recrystallization from pentane furnished 175 mg of **3** (yield 11%). Correct elemental analysis.

Received: October 20, 1986;
supplemented: November 7, 1986 [Z 1957 IE]
German version: *Angew. Chem. 99* (1987) 59

[1] O. J. Scherer, J. Schwalb, G. Wolmershäuser, W. Kaim, R. Gross, *Angew. Chem. 98* (1986) 349; *Angew. Chem. Int. Ed. Engl. 25* (1986) 363.

[2] $^{13}C\{^1H\}$-NMR (50.28 MHz, C_6D_6, TMS intern) **3**: $\delta = 90.6$ (s; C_5Me_5), 10.6 (s; CH_3); **4**: $\delta = 78.5$ (s; C_5Me_5), 9.8 (s; CH_3). EI-MS (70 eV) of **3**: m/z 346 ($M^{\oplus}$, $I_{rel} = 100\%$), 284 ($M^{\oplus} - P_2$, 91%), P_4 (19.8%), P_3 (7.9%), P_2 (53%), P (7.8%) and further, weak intensity lines.

[3] Cf.: J. L. Robbins, N. Edelstein, B. Spencer, J. C. Smart, *J. Am. Chem. Soc. 104* (1982) 1882.

[4] F. Mathey, *Struct. Bonding (Berlin) 55* (1983) 153.

[5] M. Baudler, *Phosphorus Sulfur*, in press; M. Baudler, D. Düster, D. Ouzounis, *Z. Anorg. Allg. Chem.*, in press.

[6] Cf. also the theoretical studies on $N_5^{\ominus}$ and its complex stabilization. M. T. Nguyen, M. Sana, G. Leroy, J. Elguéro, *Can. J. Chem. 61* (1983) 1435; M. T. Nguyen, M. A. McGinn, A. F. Hegarty, J. Elguéro, *Polyhedron 4* (1985) 1721.

[7] D. Catheline, D. Astruc, *Organometallics 3* (1984) 1094, and references cited therein.

Fig. 2. A contemporary article [6].

tury ago are easily made, in a flash revealing their identity to knowledgeable us. All communicated, with better graphics and computer typesetting, in a flashier journal, printed probably on poorer paper. But essentially in the same form. Is that good, is that bad?

Well, I think both. The periodical-article system of transmitting knowledge has worked remarkably well for two centuries or more. But I think there are real dangers (to which I will return) implicit in its current canonical form. My primary concern is what is really going on in the writing and reading of a scientific article, which is much more than just communication of facts. To set the stage for a discussion of the journal article, I need to say something about what I think science, chemistry in particular, is.

A Personal View of Chemistry

No one else's than my own, and others will see it in a different way:[8]

1. Science is the acquisition of knowledge about the world

That sense is clear in the etymology of the English word, or in the German *Wissenschaft* or *Naturwissenschaft.* Note that "truth" doesn't enter explicitly into that etymology. To be sure, reproducibility, verifiability, reliability, which are essential to any scientific enterprise, depend on *honest* measurement. Scientists would like to think that they acquire truth (morally and ethically valued) and not just knowledge (quite neutral; recall the tree of knowledge of good and evil in Genesis). But I would warn my colleagues that to purvey to the world at large the image of scientists as seekers of truth, rather than reliable knowledge,[9] is dangerous. It makes us out as priests, with the attendant hazards. I suspect much of the exaggerated interest of the public in the rare cases of fraud in science bears some similarity to the prurient interest of the world at large in the moral failings of priests and ministers. I think we gain knowledge, and do that as truthfully as possible.

2. Science is part discovery, part creation

I take discovery in the sense of revealing some perhaps obscured laws of nature, creation in the sense of making new things. In describing their work most scientists will stress the discovery metaphor, while most artists will emphasize creation. Well, I think much of what we do in science is creation. Especially so in chemisty. The synthesis of molecules not present on earth before is clear evidence of this. Synthesis is a marvelous congeries of discovery and creation that brings chemistry close to the arts— and to engineering.[10]

3. Science is done by human beings and their tools

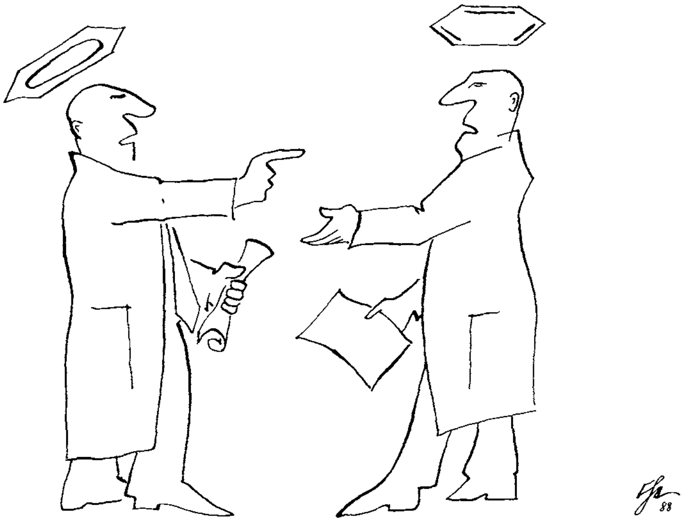
Which means that it is done by fallible human beings. The driving forces for acquiring knowledge are, to be sure, curiosity and altruism, rational motives. But creation is just as surely rooted in the irrational, in the dark, murky waters of the psyche, where fears, power, sex, childhood traumas swim in all their hidden, mysterious movements. And spur us on. To follow *Pushkin*'s *Mozart and Salieri* or its modern reincarnation in *Peter Shaffer*'s play *Amadeus* and the movie based on it: Angelic music (read chemistry) is brought into this world by such crass vessels. Not only do character and deep-down motivations not matter—their "unsavory" side may well be the driving force of the creative act.

4. Science proceeds in part by the rules

The modern model of the scientific method, associated in this century perhaps with the name of *Karl Popper*, begins with measurable, reproducible observations. One then forms alternative hypotheses or models, explaining these observations. Finally, with the aid of further experiments or reliable theory, the hypotheses are culled, eliminated one by one, until the one most likely to be right remains. Sometimes it works this way,[11] though rather interestingly this happens mostly with everyday and not ground-breaking science. But does the model apply to a modern synthesis of an unnatural molecule, for instance dodecahedrane, a beautiful $C_{20}H_{20}$ molecule shaped like its name? Or the development of the technique of nuclear magnetic resonance, equally useful to chemists seeking the arrangement of atoms in space and to a physician looking for a brain tumor?

5. Science depends on argument

"Argument" has several meanings—it could be taken as a simple process of reasoning, a statement of fact; the word also may mean disagreement, the confrontation of opposites. I would argue that both senses are essential to science: dispassionate logical reasoning *and* impassioned conviction that one (model, theory, measurement) is right and another is wrong. I feel that scientific creativity is rooted in the inner tension, within one and the same person, of knowing that he or she is right and knowing that



that conviction has to be proven to others' satisfaction. By a journal article.

6. *As a system, science works*

Individual scientists struggle to acquire knowledge, and in their struggle they are driven by many complex motivations. Because researchers are human, they are subject not only to inaccuracy, but sometimes prejudice. Remarkably, the error and prejudice of individual chemists does not matter to the progress of chemistry. Chemistry as a science, the collective activity of the half-million people in the world who are chemists, advances despite mistakes by individual chemists.[12] The science has self-correcting features in abundance: the most important one is that the more interesting the observation or theory, the more likely it is to be checked by someone else. Often for entirely the "wrong" reasons—driven by plain disbelief arising from the conviction that the initial observation must be wrong. It doesn't matter why an individual chemist repeats a critical synthesis, or tries an alternative theory. Chemistry progresses.

And yet, that a chemist *try* to prove someone else's mechanism wrong, or to make a molecule first, does matter. For without the human impulse nothing would get accomplished. It's a curious creation, this science of ours—an incredibly sturdy, exciting, and useful system of knowledge built by imperfect people, and depending for progress on their imperfection.

7. *Chemistry is the science of molecules*

Need I say more? There are limitations to the definition, but molecules, from diatomics to carbonic anhydrase and $YBa_2Cu_3O_{7-x}$ are our business. They're also big business—there are 10^{11} kilograms of sulfuric acid made per year around the world, and more pounds of ammonia than there are human beings.

8. *Chemistry is not reducible to physics*

Reductionism is something we've been saddled with for two centures. By the term I mean the setting up of a hierarchical ordering of the sciences: social sciences, biology, chemistry, physics, and a corollary definition of understanding in one science as a reduction to the next, deeper level.[13] My feeling is that scientists buy this as an ideology, but it does not represent the reality of productive work in any science, and the idea is dangerous. I'll come back to the dangers later. What I think happens in reality is that from every activity of human beings there evolves a set of objects, questions and concepts. We might call these categories. Understanding may be defined vertically, in a reductionist way, but also horizontally, in terms of the concepts and questions of that science. Most of the useful concepts of chemistry (for the chemist: aromaticity, the concept of a functional group, steric effects, and strain) are imprecise. When reduced to physics they tend to disappear.[14] But with them marvelous chemistry has been—is—wrought.

What Really Goes on in a Chemical Paper

One could proceed and list other points of view on science and chemistry, but for me these suffice to begin a discussion of the chemical article and what transpires in it.

On the face of it the article purports to be a communication of facts, perhaps a discussion, always dispassionate and rational, of alternative mechanisms or theories, and a more or less convincing choice between them. Or the demonstration of a new measurement technique, a new theory. And, remarkably, the article works. An experimental procedure detailed in *Angewandte Chemie* in German or English can be reproduced (actually how easily it can be reproduced is another story[15]) by someone with a rudimentary knowledge of either language, working in Okazaki or Krasnoyarsk. This underlying feature of potential or real reproducibility is to me the ultimate proof that science is reliable knowledge.[16]

But in so many ways there is more than meets the eye in the scientific article. I see in it the following themes, many of which are also described and analyzed in a much deeper way in a remarkable forthcoming book by *David Locke, Science as Writing*.[17]

Art

The chemical article is an artistic creation. Let me expand on what might be viewed as a radical exaggeration. What is art? Many things to many people. One aspect of art is aesthetic, another that it engenders an emotional response. In still another attempt to frame an elusive definition of that life-enhancing human activity, I will say that art is the seeking of the essence of some aspect of nature or of some emotion, by a human being. Art is constructed, human and patently unnatural.

What is written in a scientific periodical is not a true and faithful representation (if such a thing were possible) of what transpired. It is not a laboratory notebook, and one knows that that notebook in turn is only a partially reliable guide to what took place. It is a more or less (one wishes more) carefully constructed, man- or woman-made *text*. Most of the obstacles that were in the way of the synthesis or the building of the spectrometer have been excised from the text. Those that remain serve the rhetorical purpose (no weaker just because it's suppressed) of making us think better of the author. The obstacles that are overcome highlight the success story.

The chemical article is a man-made, constructed abstraction of a chemical activity. If one is lucky, it creates an emotional or aesthetic response in its readers.

Is there something to be ashamed of in acknowledging that our communications are not perfect mirrors, but in substantial part literary texts? I don't think so. In fact, I think that there is something exquisitely beautiful about our texts. These "messages that abandon", to paraphrase *Jacques Derrida*,[18] indeed leave us, are flown to careful readers in every country in the world. There they are read, in their original language, and understood; there they give pleasure *and*, at the same time, they can be turned into chemical reactions, real new things. It would be incredible, were it not happening thousands of times each day.

History

One of the oft cited distinguishing features of science, relative to the arts, is the more overt sense of chronology in science. It is made explicit in the copious use of references. But is it real history, or a prettified version?

A leading chemical style guide of my time admonished: "... one approach which is to be avoided is narration of the whole chronology of work on a problem. The full story of a research may include an initial wrong guess, a false clue, a misinterpretation of directions, a fortuitous circumstance; such details possibly may have entertainment value in a talk on the research, but they are probably out of place in a formal paper. A paper should present, as directly as possible, the objective of the work, the results, and the conclusions; the chance happenings along the way are of little consequence in the permanent record."[19]

I am in favor of conciseness, an economy of statement. But the advice of this style guide, if followed, leads to real crimes against the humanity of the scientist. In order to present a sanitized, paradigmatic account of a chemical study, one suppresses many of the truly creative acts. Among these are the "fortuitous circumstance"—all of the elements of serendipity, of creative intuition at work.[20]

Taken in another way, the above prescription for good scientific style demonstrates very clearly that the chemical article is *not* a true representation of what transpired or was learned, but a constructed text.

Language

Scientists think that what they say is not influenced by the language they use, meaning both the national language (German, French, Chinese) and the words within that language. They think that the words employed, providing they're well-defined, are just representations of an underlying material reality which they, the scientists, have discovered or mathematicized. Because the words are faithful representations of that reality they should be perfectly translatable, into any language.

That position *is* defensible—as soon as the synthesis of the new high-temperature superconductor $YBa_2Cu_3O_{7-x}$ was described, it *was* reproduced, in a hundred laboratories around the globe.

But the real situation is more complex. In another sense words are all we have. And the words we have, in any language, are ill-defined, ambiguous. A dictionary is a deeply circular device—just try and see how quickly a chain of definitions closes upon itself. Reasoning and argument, so essential to communication in science, proceed in words. The more contentious the argument, the simpler and more charged the words.[21]

How does a chemist get out of this? Perhaps by realizing what some of our colleagues in linguistics and literary criticism learned over the last century.[22] The word is a sign, a piece of code. It signifies something, to be sure, but what it signifies must be decoded or interpreted by the reader. If two readers have different decoding mechanisms, then they will get different readings, different meanings. The reason that chemistry works around the world, so that BASF can build a plant in Germany or Brazil and expect it to work, is that chemists have in their education been taught the same set of signs.

I think this accounts in part for what *Carl Friedrich von Weizsäcker* noted in a perceptive article on "The Language of Physics":[23] If one examines a physics (read chemistry) research lecture in detail one finds it to be full of imprecise statements, incomplete sentences, halts, etc. The seminar is usually given extemporaneously, without notes, whereas humanists most often read a text verbatim. The language of physics or chemistry lectures is often imprecise. Yet chemists understand those presentations (well, at least some do). The reason is that the science lecturer invokes a code, a shared set of common knowledge. He or she doesn't have to complete a sentence—most everyone knows what is meant halfway through that sentence.

Graphics

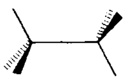
The semiotics of chemistry is most apparent in the structures of molecules that grace most every page of a chemical journal, that identify at a glance a paper as chemical.[24,25] The given, just over a century old, is that the structure of a molecule matters. It's not only what the atomic constituents are. It's also how the component atoms are connected up, how they are arranged in three-dimensional space, and how easily they move from their preferred equilibrium positions. The structure of a molecule, by which I mean the disposition in space of nuclei and electrons, both the static equilibrium structure and its dynamics, determines every physical, chemical, and ultimately biological property of the molecule.

It is crucial for chemists to communicate three-dimensional structural information to each other. The media for that communication are two-dimensional—a sheet of paper, a screen. So one immediately encounters the problem of representation.

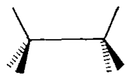
Actually that problem is already there. What is a ball-and-stick model of a molecule? Is that reality? Of course not. The model is just one representation of the equilibrium positions of the nuclei, with some further assumptions about bonding. An instructive videotape from the laboratory of *F. P. Brooks, Jr.* at the University of North Carolina is entitled "What Does a Protein Look Like?" It shows 40 different representations (recalling to my mind the woodcut suite of *Hokusai* entitled "36 Views of Mt. Fuji") of one and the same enzyme, superoxide dismutase—a "ball-and-stick" model, a "space-filling" model, the electrostatic field experienced by a probe charge near the molecule, and so on.[26]

Let me return to the communication problem. Chemists are impelled to communicate three-dimensional information in two dimensions. But they're not *talented* at that. Young people are not selected or select themselves to be chemists on the basis of their artistic ability.

So people are required to do what they're not talented at. That's one definition of life! Chemists cope, by the expedient of inventing a code for communicating three-dimensional structure. *And* they train people in that code. The various elements of that code are known to chemists as Fischer or Newman projections, or as the wedge-dash representation. A molecule of ethane, C_2H_6, is represented in two possible geometries, **1** and **2**.


staggered

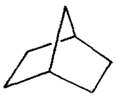
1

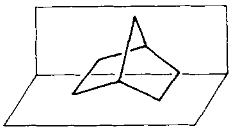

eclipsed

2

Note another piece of code: carbon is that vertex of the graph which has four lines to it, but it's not labeled C. There are hydrogens at the ends of the lines. They're also not labeled. The notation is simple: a solid line is in the plane of the paper, a wedge in front, a dashed line in back. Saying that may be enough to make these structures rise from the page for some people, but the neural networks that control representation are effectively etched in, for life, when one handles (in human hands, not in a computer) a ball-and-stick model of the molecule while looking at this picture.

It's fascinating to see the chemical structures floating on the page of every journal and to realize that from such minimal information people can actually *see* molecules in their mind's eyes. The clues to three-dimensionality are minimal. The molecules do float, and you're usually discouraged from putting in a reference set of planes to help you see them (**3** vs. **4**).

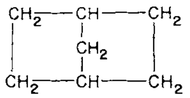

3


4


5

Some chemists rely so much on the code that they don't draw **3** but **5**. What's the difference? One line "crossed" instead of "broken". What a trivial clue to three-dimensional reconstruction, that one part of a molecule is behind another one, is given in **3**, absent in **5**! The person who draws **5** is making many assumptions about his audience. I bet he or she hardly thinks about that.

The policies of journals, their economic limitations, and the available technology put constraints not only on what is printed but also on how we *think* about molecules. Take norbornane, C_7H_{12}, molecule **3**. Until about 1950 no journal in the world was prepared to typeset this structure as **3**. Instead you saw it in the journal as **6**. Now everyone



6

knew, since 1874, that carbon was tetrahedral, meaning that the four bonds to it were formed along the four directions radiating out from the center of a tetrahedron to its vertices. You can see this geometry in the two carbon atoms of structures **1** and **2**. Molecular models were available or could be relatively easily built. Yet I suspect that the image or icon of norbornane that a typical chemist had in his mind around 1925 was **6** and not **3**. He was conditioned by what he saw in a journal or textbook—an image. He was moved to act, in synthesizing a derivative of this molecule, for instance, by that unrealistic image.

Maybe it's not that different from the way we approach romance in our lives, equipped with a piecewise reliable set of images from novels and movies.

Style

Every manual of scientific writing I've seen exhorts you to use an impersonal, agentless, superrational style. Please give us the facts, gentlemen, and just the facts! Still style rears its head.

My papers are recognizable in a journal just by the proportion of the space given to graphical material, or the way I "line" my orbitals. *R. B. Woodward*'s papers were recognizable in the (constructed) elegance of their scientific storyline, and in the matching elegance, the cadence of his words. I can read a paper by *Jack Dunitz*, by *Rolf Huisgen*, *Rudolf Hoppe*, or *Bill Doering* and hear their voices in these papers just as surely as I hear the voice of *A. R. Ammons*, a great American poet, or of *Bertolt Brecht*, a German one, when I see their work on a printed page.

It is in the nature of creative human beings to have a style. Why should I write my theory the way *Bill Goddard*, a theorist I admire, does, anymore than you expect *Karlheinz Stockhausen* and *Pierre Boulez* to write piano pieces that sound alike?

Dialectical Struggles

A nice, even-toned, scientific article may hide strong emotional undercurrents, rhetorical maneuvering, and claims of power. One has already been mentioned—the desire to convince, to scream "I'm right, all of you are wrong", clashing with the established rules of civility supposedly governing scholarly behavior. Where this balance is struck depends on the individual.

Another dialogue that is unvoiced is between experiment and theory. There is nothing special about the love-hate relationship between experimentalists and theorists in chemisty. You can substitute "writer" and "critic" and talk about literature, or find the analogous characteristics in economics. The lines of the relationship are easily caricatured—experimentalists think theorists are unrealistic, build castles in the sky. Yet they need the frameworks of understanding that theorists provide. Theorists may distrust experiments, wish that people would do that missing experiment, but where would the theorists be without any contact with reality?

An amusing manifestation of the feelings about this issue is to be found in the occasionally extended quasi-theoretical discussion sections of experimental papers. These

sections in part contain a true search for understanding, but in part what goes on in them is an attempt to use the accepted reductionist ideal (with its exaggerated hailing of the more mathematical)—so as to impress one's colleagues. On the other side, I often put more references to experimental work in my theoretical papers than I should, because I'm trying to "buy credibility time" from my experimental audience. If I show experimental chemists that I know of their work, perhaps they'll give me a little time, listen to my wild speculations.

Another struggle, related, is between pure and applied chemistry. It's interesting to reflect that this separation also may have had its roots in Germany in the mid-nineteenth century; it seems to this observer that in the other chemical power of that time, Britain, the distinction was less congealed. Quite typical in a pure chemical paper is a reaching out after some justification in terms of industrial use. But at the same time there is a falling back, an unwillingness to deal with the often unruly, tremendously complicated world of, say, industrial catalysis. And in industrial settings there is a reaching after academic credentials (quite typical, for instance, of the leaders of chemical industry in Germany).

The Id Will Out

I use the subject word in the psychoanalytical sense, referring to the complex of instinctive desires and terrors that inhabit the collective unconscious. On one hand, these irrational impulses, sex and aggression figuring most prominently, are our dark side. On the other hand, they provide the motive force for creative activity.[27]

The irrational seems to be effectively suppressed in the written scientific word. But of course scientists are human, no matter how much they might pretend in their articles that they are not. Their inner illogical forces push out. Where? If you don't allow them in the light of day, on the printed page, then they will creep out or explode in the night, where things are hidden, and no one can see how nasty you are. I refer, of course, to the anonymous refereeing process, and the incredible irrational responses unleashed in it by perfectly good and otherwise rational scientists. You have to let go sometime...

I actually think that what saves the chemical article from dullness is that its language comes under stress. We are trying to communicate things that perhaps cannot be expressed in words but require other signs—structures, equations, graphs. And we are trying hard to eliminate emotion from what we say. Which is impossible. So the words we use occasionally become supercharged with the tension of everything that's *not* being said.

...

So, many things go on in a scientific article. I will spare you the charts that I've seen hanging in many laboratories, that translate shop-worn phrases into what they really mean. Like "A regime of slow cooling over a period of four weeks produced a 90% yield of black crystals of...", meaning "I went on vacation and forgot to wash out the flask. When I came back..." And so on.

I want to return to the complexity of deciding what is truth in the scientific process. In a recent article, *Harald Weinrich*[28] describes the classic paper of *Watson* and *Crick* on the structure of DNA in *Nature* in 1953. It is succinct, beautifully reasoned, elegant. *David Locke*, in his book, analyzes the rhetorical structure and the use of irony in the same paper.[17] I think most readers were immediately convinced that the Watson and Crick model was the truth, that this was the way it had to be. And so it is (with some minor variation on hydrogen-bonding schemes in unusual forms of DNA). The Watson and Crick model was and is right. One needs little more.

But then in 1968 *Watson* writes a book, *The Double Helix*, in which he tells the story of how it really happened. Of course, it's a self-centered story, and not kind or fair to *Rosalind Franklin* and others. *Watson*'s story is much like one of the four views of an event in *Akira Kurosawa*'s masterful film *Rashomon*. It needs other views, which some historians have provided. But there is no question that *Watson*'s account is vibrant, full of life. It tells us how he saw the truth, and I think it's a great book.

So (and here I follow *Weinrich*) what *is* the truth: Is it the 1953 paper of *Watson* and *Crick*, or is it the 1968 book by *Watson*? Does the latter diminish the former? It bears reflection.

What Is to Be Done?

I have tried to deconstruct, to borrow some language from critical theory, the scientific article, ossified in its present form for over a hundred years. I think I could have done this better with a specific text before me, but then I would have run the danger of libel suits or loss of friendship. And it is in the nature of human beings to be unable to criticize, truly, deeply, their own work. So I can't do it to myself. But I'm sure every chemist knows some superb example of what I allude to, especially in the work of one of his less favorite scientists.

The deconstruction is done by me not with malice, but with care. I love this molecular science. I love its richness, and the underlying simplicity, but most of all the rich, life-giving variety and connection of all of chemistry. Let me give you an example in Figure 3. I see C_2 in a carbon arc and in the tail of Halley's Comet.[29a] I see it in acetylene, ethylene, and ethane. I see it in the lovely molecular complexes of *P. Wolczanski*,[29b] *M. I. Bruce*,[29c] and *G. Lon-*

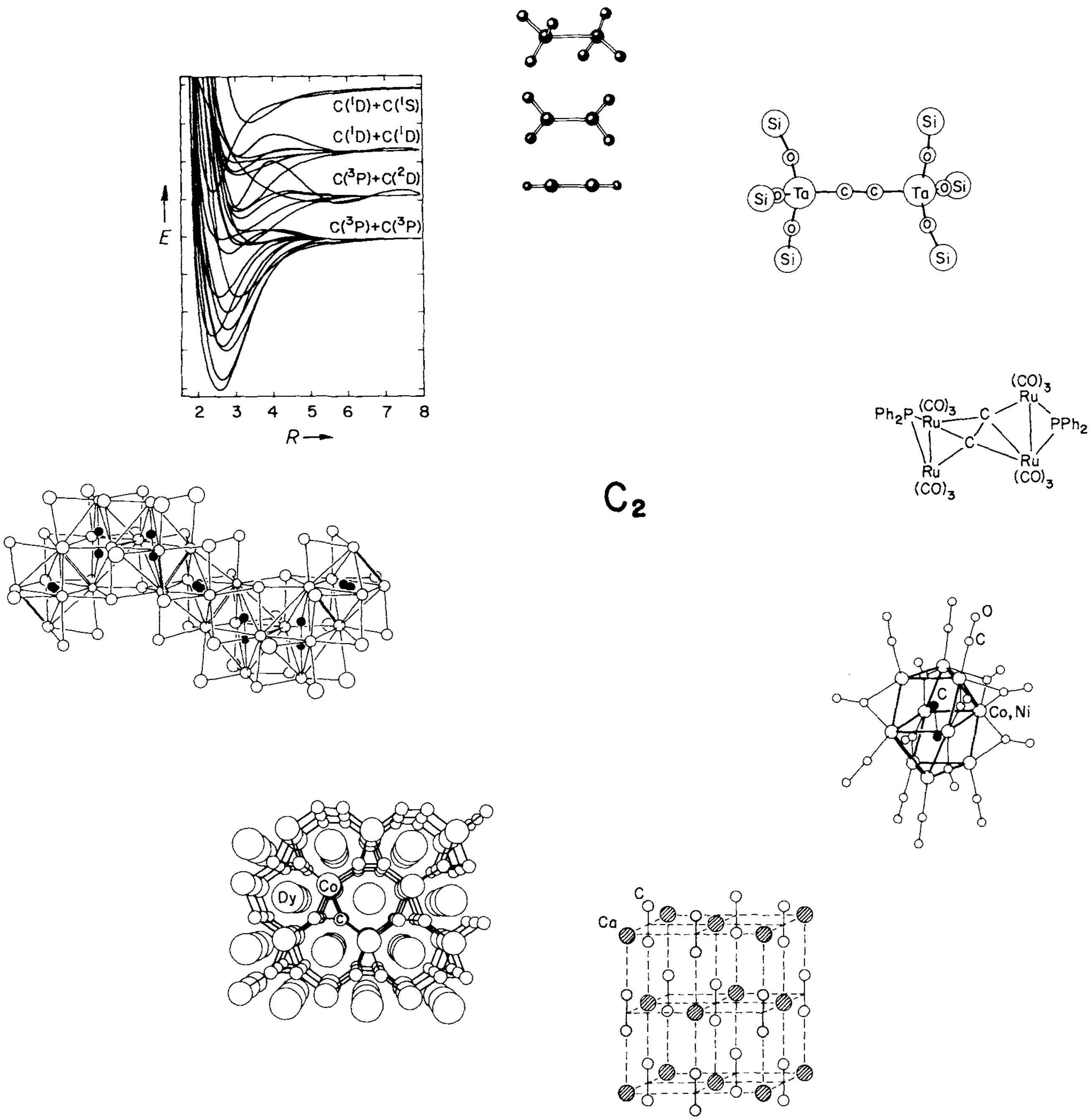


Fig. 3. Some of the ways in which C_2 finds its way in this world. Clockwise from 10:30: a) some calculated potential energy curves for diatomic C_2 [29a]; b) ethane, ethylene, acetylene; c) a dinuclear tantalum complex of C_2 [29b]; d) Ru_4C_2 cluster [29c]; e) C_2 inside a Co_3Ni_7 cluster [29d]; f) calcium carbide; g) $DyCoC_2$ [29e]; h) $Gd_{12}C_6I_{17}$ [29f].

goni[29d] and their co-workers, shown in Figure 3. I see it in CaC_2, in *W. Jeitschko*'s[29e] and *A. Simon*'s[29f] and their co-workers' rare-earth carbides. It's staggering!

I know that that richness was created by human beings. So I'm unhappy to see their humanity suppressed in the way they express themselves in print. I also think that there are some real dangers in the present intellectual stance of scientists and in their ritual mode of communication.

Here are the dangers as I perceive them. Acceptance of a facile reductionist philosophy, a vertical mode of understanding appropriated as the *only* mode of understanding, creates a gap between us and our friends in the arts and humanities. They know very well that there isn't only one way of "understanding" or dealing with the death of a parent, or a political election, or a woodcut by *Ernst Ludwig Kirchner*. The world out there is refractory to reduction, and if we insist that it must be reducible, all that we do is to put ourselves into a nice box. The box is the small class of problems that are susceptible to a reductionist understanding.

A second danger, more specific to the scientific article, is that by dehumanizing our mode of communication, by removing emotion, motivation, the occasionally irrational, we may have in fact done much more than chase away the

Natural Philosophers. That we've accomplished, to be sure. But 150 years down the line what we have created is a mechanical, ritualized product that 3×10^5 times per year propagates the notion that scientists are dry and insensitive, that they respond only to wriggles in a spectrum. The public at large types us by the nature of our product. How can it do otherwise when we do not make a sufficient effort to explain to the public what it is that we really do in our jargon-barricaded world?

What is to be done? I would argue for a general humanization of the publication process. Let's relax those strictures, editorial or self-imposed, on portraying in words, in a primary scientific paper, motivation, whether personal and scientific, emotion, historicity, even some of the irrational. So what if it takes a little more space? We *can* keep up with the chemical literature, and tell the mass of hack work from what is truly innovative, without much trouble as it is. The humanizing words will not mislead; they may actually encourage us to read more carefully the substance of what is said. I would plead for a valuation and teaching of style, in the written and spoken language of one's own country, as well as in English. I think chemistry has much to gain from reviving the personal, the emotional, the stylistic core of the struggle to discover and create the molecular world.

Received: March 13, 1988 [A 701 IE]
German version: *Angew. Chem. 100* (1988) 1653
Cartoons: *Constance Heller*

[1] *Angewandte Chemie* has been very important to me personally, and it is a pleasure for me to dedicate this lecture to the past and present editorial staffs of one of the world's greatest journals.
[2] E. Garfield: *Essays of an Information Scientist*, ISI Press, Philadelphia 1981, pp. 394-400 and references therein.
[3] a) S. Shapin, *Social Stud. Sci. 14* (1984) 487; b) P. Dear, *Isis 76* (1985) 145; c) F. L. Holmes in P. Dear (Ed.): *The Paper Laboratory*, University of Pennsylvania Press, Philadelphia, in press.
[4] F. Goldmann, *Ber. Dtsch. Chem. Ges. 21* (1888) 1176.
[5] For a discussion of the evolution of science writing see B. Coleman, *New York Times Book Review*, September 27, 1987, p. 1; also R. Wallsgrove, *New Sci. 116* (1987) No. 24, p. 55.
[6] O. J. Scherer, T. Brück, *Angew. Chem. 99* (1987) 59; *Angew. Chem. Int. Ed. Engl. 26* (1987) 59.
[7] The version shown here is in English. Angewandte Chemie is unique in printing (since 1963) the same article in English and German versions.
[8] For a demonstration of the range of attitudes about what science is, see the discussion in the pages of *Nature* (*330* (1987) 308, 689; *331* (1988) 129, 558; following an article by *T. Theocharis* and *M. Psimopoulos* (*Nature 329* (1987) 595).
[9] The phrase is used after J. Ziman: *Reliable Knowledge*, Cambridge University Press, Cambridge, England 1978. I disagree with some points in this book, but there is no better, nor more humanistic, description of what science is and should be than this small volume.
[10] M. Berthellot: *Chimie Organique Fondée sur la Synthèse, Tome 2*, Mallet-Bachelier, Paris 1860. See also J.-P. Malrieu, *L'Actualité Chimique 1987*, No. 3, p. IX; A. F. Bochkov, V. A. Smit: *Organicheskii Sintez* (Organic Synthesis), Nauka, Moscow 1987; and an essay "*In Praise of Synthesis*" by R. Hoffmann, to be published.
[11] For different views of the way science works see a) P. Feyerabend: *Against Method*, NLB, London 1975; *Wider den Methodenzwang*, Suhrkamp, Frankfurt am Main 1976; b) B. Latour, S. Woolgar: *Laboratory Life*, Princeton University Press, Princeton 1986; c) K. Knorr-Cetina: *Die Fabrikation von Erkenntnis*, Suhrkamp, Frankfurt am Main 1984.
[12] I was reminded of the importance of the individual-system distinction through a conversation with *Barry Carpenter*. I'm grateful to him for a discussion of the points raised in this essay, as well as to another colleague, *Bruce Ganem*, for his comments.
[13] Several types of reductionism must be distinguished. See the interesting debate between *S. Weinberg* (*Nature 330* (1987) 443; *331* (1988) 475) and *E. Mayr* (*Nature 331* (1988) 475 and references therein).
[14] See, inter alia, K. Mislow, P. Bickart, *Israel J. Chem. 15* (1976/77) 1; D. W. Theobald, *Chem. Soc. Rev. 5* (1976) 203.
[15] *R. G. Bergman*, in an unpublished lecture on "Values in Science", cites some fascinating raw data on this question, coming from the experience of the journals *Organic Synthesis* and *Inorganic Synthesis*.
[16] *Latour* and *Woolgar* ([11b], p. 183) are rather scornful of the kind of marveling at verification and reproducibility of scientific facts that I engage in here. I think they've gotten caught in the consistently questioning and skeptical ideology of their otherwise incisive anthropological investigation of how scientific facts are constructed. They should take a look at the systematic, worldwide, industrial production of pharmaceuticals, just to take one example of a reproducible experimental activity.
[17] D. Locke: *Science as Writing*, to be published.
[18] J. Derrida in his essay "Signature Event Context" in *Marges de la Philosophie*, Editions Minuit, Paris 1972, pp. 365-393; translation (by A. Bass): *Margins of Philosophy*, University of Chicago Press, Chicago 1982, pp. 307-330.
[19] L. F. Fieser, M. Fieser: *Style Guide for Chemists*, Reinhold, New York 1960, pp. 51-52.
[20] P. B. Medawar, *Saturday Review*, August 1, 1964, p. 42, also argues that the standard format of the scientific article misrepresents the thought processes that go into discovery.
[21] See R. Hoffmann, *Am. Sci. 75* (1987) 619; *76* (1988) 182.
[22] For an introduction to modern literary theories see T. Eagleton: *Literary Theory*, University of Minnesota Press, Minneapolis 1983.
[23] C. F. von Weizsäcker: *Die Einheit der Natur*, dtv, Munich 1974, pp. 61-83.
[24] For a description of the geometrical and topological information processing that goes on in organic chemistry, see also N. J. Turro, *Angew. Chem. 98* (1986) 872; *Angew. Chem. Int. Ed. Engl. 25* (1986) 882.
[25] *Pierre Laszlo* has written an illuminating article on technical illustration ("The Pictures of Science") that is relevant to my discussion. A French version of this article ("Science en images") has been accepted for publication in *ECALE*, No. 2, published by Ecole Cantonale d'Art, Lausanne.
[26] M. Pique, J. S. Richardson, F. P. Brooks, Jr., *Invited Videotape, 1982 SIGGRAPH Conference*. I am grateful to *J. S. Lipscomb* for showing this videotape to me.
[27] *P. B. Medawar* says, along the same lines, that "scientists should not be ashamed to admit ... that hypotheses appear in their minds along uncharted by-ways of thought ..." (see [20]).
[28] H. Weinrich, *Merkur 39* (1985) No. 436, p. 469. I'm grateful to *P. Gölitz* for bringing this paper to my attention.
[29] a) The C_2 potential energy curves are drawn after *P. P. Fougere* and *R. K. Nesbet* (*J. Chem. Phys. 44* (1966) 285; b) $[\{(t\mathrm{Bu_3SiO})_3\mathrm{Ta}\}_2\mathrm{C_2}]$: R. E. LaPointe, P. T. Wolczanski, J. F. Mitchell, *J. Am. Chem. Soc. 108* (1986) 6382; c) $[\mathrm{Ru_4C_2(PPh_2)_2(CO)_{12}}]$: M. I. Bruce, M. R. Snow, E. R. T. Tiekink, M. L. Williams, *J. Chem. Soc. Chem. Commun. 1986*, 701; d) $[\mathrm{Co_3Ni_7C_2(CO)_{15}}]^{3\ominus}$: G. Longoni, A. Ceriotti, R. Della Pergola, M. Manassero, M. Perego, G. Piro, M. Sansoni, *Phil. Trans. R. Soc. London, Ser. A 308* (1982) 47; e) $\mathrm{DyCoC_2}$: W. Jeitschko, M. H. Gerss, *J. Less. Common Met. 116* (1986) 147; f) $\mathrm{Gd_{12}C_6I_7}$: A. Simon, E. Warkentin, *Z. Anorg. Allg. Chem. 497* (1983) 79.