Alfred Bader fonds

Correspondence - General

Hoffman, Roald
1995-96

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A Chemist Helping Chemists

November 22, 1996

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Professor Hoffmann:

Thank you for your phone message, which I have relayed to Dr. Bader. He and Isabel are presently at their English home through early January.

He did, however, suggest that I send you the enclosed photo of a *Joseph Sold Into Slavery* which he owns. It was painted by a Rembrandt student, Sibilla, and is oil on panel. He says it is an excellent representation, even if it doesn't have camels. If this photo will work, I do have slides as well, which might be easier to reproduce. If it doesn't meet your needs, please return the photo at your convenience.

Best wishes,

Cheryl Weiss
Office Manager

Cornell University
Department of Chemistry
Baker Laboratory
Ithaca, New York 14853-1301 USA

3/8/97

Dear Alfred:

Another art research question:
You gave me once a lovely volume, the Rachel Wischnitzer "From Dura to Rembrandt"). And in our book we have used an image from that book, an engraving of the Ordeal of Bitter Waters by C.N. Schurtz in J C Wagenseil's Sotah (Altdorf, 1674).

I've photographed from the book but I think it might come out better from an original. I'm about to go to the library to check where this rare book is in the US, but I thought I might also ask you, just in case you have a slide. Please don't go to any trouble, just tell me if you have it. (It's on p. 156 of Wischnitzer book)

I wish I had known her.

Roald

Hoffmann

Cornell University

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Ithaca, New York 14853-1301 USA

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TO: Alfred Bader

FAX NUMBER: 414-277-0709

Number of pages (including this page) being transmitted: 2
[Please contact **R. Hoffmann** if you didn't receive all pages.]

DATE: 3/8/97

Dr. Alfred Bader
924 East Juneau, Suite 622
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Phone: 414/277-0730
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A Chemist Helping Chemists

February 21, 1997

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

Yesterday was such a fun day. All sorts of happenings, including the sale of a great painting to one of the country's best museums. But best of all, I had the evening to look forward to, to read your wonderful Chapter Three.

Gott lebt im Detail and so I enclose a few trivial corrections which you would have caught anyway.

Baba Mezia does of course refer to Deuteronomy XXX, 12, but we hear that portion in the Torah only once a year, and Psalm 115 many times.

The story in *Baba Mezia* 84a is one of the saddest in the Talmud: The mourner went out of his mind and died. Of course it also shows that there were "yes men" even in Talmudic days.

Did you know that Loschmidt entitled the first draft of his 1861 *Chemische Studien* "Konstitutions-Formeln der organischen Chemie in geographischer Darstellung?" I suspect that was a galley proof, changed later to *Graphischer*. Probably somebody told Loschmidt that it just didn't make sense to think of depicting molecules in space and that *graphic* was better than *geo*graphic.

I enclose a copy of a brief paper on Loschmidt and Couper which appeared in last September's *Chemistry in Britain*. Of course I thanked you in footnote 19 for allowing me to use Woodward's manuscript which I hope will be published in full sometime. Note that the paper also contains an error: The Cope lecture was in 1972 not in 1973. *Gott lebt im Detail.*

Kolbe was not only unbelievably insulting, but viciously anti-semitic. But whoever wrote "too bad they don't write them like that today" should read Professor Jensen's letter to *Chemistry in Britain*, copy enclosed. Jensen was editor of the Bulletin of the division of the history of chemistry of the American Chemical Society. He wrote that letter to the editor of *Chemistry in Britain* who unfortunately refused to publish it saying that he would not publish such insulting letters.

May I ask you for your opinion in a totally different matter? I have established an award to the best young Czech organic or bio-organic described in the enclosed. As you speak Polish, surely you will understand Czech. The award was recently given to a very able man, Dr. Havlicek, whom I certainly would not consider an organic chemist or a biochemist. Dr. Drasar's letter will be self-explanatory. You probably know Havlicek's work; do you think of him as either an organic or biochemist? I have established all sorts of chemical awards, in the U.S., Canada, Britain, and in the Czech Republic, and this is the first time that this question has arisen.

Thank you again for allowing me the joy of reading Chapter Three before reading the book.

Could I not persuade you to come a visit us in Milwaukee before long?

Fond regards, as always,

AB/nik

Enclosures

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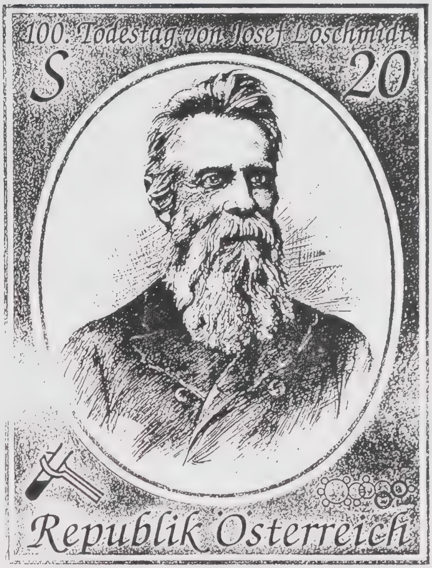
Enclosures

A chemist turns **detective**

Unlike the name of August Kekulé, the names Josef Loschmidt and Archibald Scott Couper will probably mean little to most chemists. But, as **Alfred Bader** explains, perhaps it is now time to reconsider who should take the credit for some of the great man's discoveries



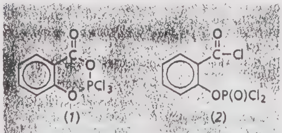
An Austrian stamp issued in 1995 in honour of Loschmidt. The structure on the bottom right is of cinnamic acid, one of Loschmidt's many correct aromatic structures

WINSTON CHURCHILL ONCE SAID that 'Men occasionally stumble over the truth, but most of them pick themselves up and hurry off, as if nothing had happened'. Fortunately, this does not apply to Richard Anschütz,[1] whose detective work includes revealing the role of Austrian schoolteacher Josef Loschmidt in predicting the circular structure of benzene (*Chem. Br.*, February, 1993, p 126). Although neither man has become a household name, some chemists may remember the Anschütz thermometer or the Loschmidt/Avogadro Number from their physical chemistry lectures. However, few of us know that Anschütz revolutionised the history of chemistry by following leads during the preparation of his biography[2] of August Kekulé published in 1929.

Testing times

August Kekulé is a household name; he was one of the most famous German chemists of the 19th century, and Anschütz was his assistant and successor as professor of organic chemistry at Bonn University. Kekulé's fame rests on two great discoveries. First, in a paper[3] in May 1858, he showed that carbon is tetravalent and that one carbon atom can be linked to another. Secondly, in 1865 he showed benzene as a cyclohexatriene[4] – a ring of six carbon atoms – an idea that he claimed 25 years later had come to him in a dream.

It was through Anschütz's researches into this latter discovery that chemists first became aware of the significance of an earlier publication by Loschmidt, and the continuing controversy[5] over who first predicted the circular structure of benzene (A. J. Rocke, *Chem. Br.*, May 1993, p 401). Less well known, but equally significant, Anschütz's persistence has also led to a question mark beside Kekulé's earlier claim to fame over the tetravalency of carbon, and brought to light the work of another virtually unknown chemist, Archibald Scott Couper.



The incorrect (*1*) and correct (*2*) product structures suggested to result from the reaction of PCl_5 and salicyclic acid

Couper's name first came to Anschütz's attention in the early 1880s, long before he started on his biography of Kekulé. At that time Anschütz was studying the reaction of salicylic acid with phosphorus pentachloride. Some great chemists, Kekulé and Kolbe among others, as well as a young Scot, Archibald Scott Couper, had previously studied this reaction. Couper claimed[6] to have obtained a phosphorus-containing compound boiling around 290 °C. Kekulé had tried[7] to repeat Couper's work over 20 times, always in vain. No one was successful until Anschütz and one of his students, George Dunning Moore, proved that Couper was correct.[8]

Couper suggested[6] that the product was a cyclic structure (*1*), one of the first heterocyclic structures ever proposed, but it took over 100 years before the alternative structure (*2*), considered probable by Anschütz,[9] was proven unambiguously by Pinkus and Waldrep.[10]

Investigating Couper

Early this century, when he began work on his biography of Kekulé, Anschütz became aware of other more important papers by Couper. The most important, entitled *On a new chemical theory*,[11] proposed the tetravalent nature of carbon and its ability to link together to form C—C bonds. Anschütz was struck by the similarity of this paper with Kekulé's prestigious paper of May 1858 on the same subject. Couper had given his paper to his French professor, Adolph Wurtz for submission to the French Academy. However, publication was delayed, perhaps because Wurtz was not yet an academy member, and the paper was not presented until June 1858, by the famous French chemist Jean Baptiste Dumas.

In the meantime, Kekulé's paper,[3] submitted on 16 March, 1858, was published in May,

The young Scottish chemist Archibald Scott Couper (1831–92)

although Couper's paper had almost certainly been submitted first.

Intrigued by the brilliance of Couper's work, Anschütz wrote to chemists he believed might have known and/or worked with him. He learned from one of Couper's former colleagues, Albert Ladenburg, that 'Couper was very angry, he questioned Wurtz and became insulting. Wurtz would not put up with that and dismissed him from his laboratory'.[12]

Righting the records

In August 1858, Kekulé had publicly attacked[13] Couper's claim to have developed a new chemical theory, saying that he had done so first and asking Dumas to note his complaint. He also wrote to Wurtz declaring that: 'As a matter of principle, I will never claim priority for theoretical views as long as that can be avoided. Also, I will not, à la Couper, sound a big horn to proclaim my views as a "nouvelle théorie chimique". I will leave it to posterity and the legal sense of others to establish whether the views belong to me and to what extent'.[14]

Anschütz believed[15] that Wurtz should have stated that Couper had given him his paper some time before Kekulé's work was published. Wurtz failed to do that. It was almost 50 years before the significance of Couper's claim began to be realised, thanks to work by Anschütz, joined by Alexander Crum Brown, professor of organic chemistry at Edinburgh University.

Their work was taken up by Leonard Dobbin, assistant to Crum Brown and later a reader at Edinburgh University. While preparing a paper on Couper, Dobbin wrote to Anschütz, who replied in December 1931:

> For Crum Brown's successful investigations about Couper's life, I was only the catalyst. Crum Brown was a doctor of medicine and had the idea to check with insane asylums about Couper; in that he succeeded.
>
> I noted with pleasure that the Scots celebrated Couper's 100th birthday from an essay *A. S. Couper of Kirkintilock: a remarkable Scots scientific centenary* in the *Journal of the Society of Chemical Industry* of May 8, 1931. To my deep regret, nothing was said therein about Crum Brown's work to discover Couper's fate.[16]

Anschtüz was not one to blow his own horn.

Dobbin's article, *The Couper quest*,[17] describes step-by-step, letter-by-letter, how Anschütz enlisted the help of Crum Brown to find out about Couper's life, family and final illness. He includes a letter of July 1906 to Crum Brown from Couper's German friend, Gustav Berring who stated: 'Couper afterwards wrote to me from Paris that he had made a discovery which Professor Kekulé in Heidelberg also claimed for himself, although wrongly since priority undoubtedly belonged to him (Couper)'.

My own interest in Couper[18] began as a student at Harvard, when I first heard about him from Robert Burns Woodward, who knew Anschütz's biography and *The Couper quest*. Woodward later made clear his views during a Cope award lecture[19] in 1973:

> In 1858, Archibald Scott Couper was a 27-year-old Scotsman, studying chemistry in the laboratory of Adolph Wurtz in Paris. He had toyed with philosophy and architecture before settling down to chemical studies. Having pursued the latter for, I believe, something on the order of little more than a year, he prepared a paper entitled *On a new chemical theory*, which, after some delay, was published in the *Comptes rendus* of the French Academy of Sciences. In that literally astonishing paper, one may see presented, for the first time, structural formulae, identical with those we use today – and these are, of course, the most fundamental theoretical tools of organic chemistry.
>
> Now, August Kekulé is rightly given credit for his recognition of and insistence upon the quadrivalency of carbon, and for his brilliant later proposal of the structure of benzene. [Unfortunately, Woodward was unaware of Loschmidt's work]. But he was not, as many believe, the father of structural chemistry. Indeed, in his famous 1858 paper *On the constitution and metamorphoses of chemical compounds and the chemical nature of carbon*, he makes very clear his belief at that time that chemical substances adopted diverse structures in response to the influence of attacking reagents; and for many years thereafter, he continued to use, in his own papers, the cumbersome and often obscure 'type' formulae of Gerhardt and Laurent. He was, in truth, too much under the influence of the theoretical and physical chemists of the time, who were inordinately opposed to the idea of fixed chemical structure – so much so that, until 1886, the infant *Berichte d. Deutschen Chemischen Gesellschaft*, born in 1868, would only print structural formulae using dotted-and-dashed lines; the use of solid lines to represent nearest-neighbour relationships would have imputed too much reality to an hypothesis which leading theorists of the day simply would not accept.
>
> So, Archibald Scott Couper deserves recognition for the introduction of structural formulae as we know them ...

Woodward surmised that:

> Couper has received little credit for his brilliant contribution, no doubt largely because not long after his paper was published, he returned to his mother's home in Scotland, went mad, and played no further role in chemistry'.

We cannot tell whether Couper's mental illness was triggered largely by his expulsion from Wurtz's laboratory or by a subsequent sunstroke, but certainly Anschütz was correct when he ended his biography of Couper with:

The inquisitive Richard Anschütz (1852–1937)

'In the history of organic chemistry, the sorely tried Archibald Scott Couper deserves a place of honour beside his more fortunate fellow-worker, Friedrich August Kekulé'.

Thanks to such publicity Couper had become sufficiently well-known to be honoured with Kekulé at the 100th anniversary of the foundation of the structural theory.[20]

Kekulé's fame rests on two pillars,[3-4] both questioned by Anschütz's detective work. Couper was silenced by his mental illness, and Loschmidt chose to remain silent. Anschütz believed[21] that this was 'because of the undemanding modesty which was an integral part of his character. The discovery of *Chemische Studien* ... he left to chance' and luckily to Richard Anschütz. Without Anschütz's persistence, we would know little about Couper's work and life and nothing about Loschmidt's chemistry.

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5. G. P. Schiemenz, *Naturwiss. Rundsch.*, 1993, **46**, 85; G. P. Schiemenz, *Sudhoffs Arch.*, 1994, **78**, 41.
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11. A. S. Couper, *Compt. rend .Acad. Sci.*, 1858, **46**, 1157.
12. R. Anschütz to A. Crum Brown, unpublished letter dated 22 July 1906.
13. A. Kekulé, *Compt. rend. Acad. Sci.*, 1858, **47**, 378.
14. R. Anschütz, *August Kekulé*, vol 1, p 158. Berlin: Verlag Chemie, 1929.
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17. L. Dobbin, *J. Chem. Ed.*, 1934, **11**, 331.
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19. Quoted from the unpublished manuscript of R. B. Woodward's August 1973 Cope lecture in Chicago, courtesy of R. Hoffmann and the Chemical Heritage Foundation.
20. H. C. Brown, *J. Chem. Ed.*, 1959, **36**, 104.
21. J. Loschmidt, *Chemische Studien I*, republished by R. Anschütz in Ostwald's *Klassiker der exakten Wissenschaften*, no. 190, p 109. Leipzig 1913; reprinted by Aldrich Chemical Co., 1989, cat. no. Z18577–9.

Chemistry

IN BRITAIN

Building conservation

Kekulé revisited

Chemicals in the North East

N 009-3106 Volume 32 Number 9 September 1996

of its place—others affirm, four hundred cubits. 'No proof can be brought from a carob-tree,' they retorted. Again he said to them: 'If the *halachah* agrees with me, let the stream of water prove it!' Whereupon the stream of water flowed backwards. 'No proof can be brought from a stream of water,' they rejoined. Again he urged: 'If the *halachah* agrees with me, let the walls of the schoolhouse prove it,' whereupon the walls inclined to fall. But R. Joshua rebuked them, saying: 'When scholars are engaged in a *halachic* dispute, what have ye to interfere?' Hence they did not fall, in honour of R. Joshua, nor did they resume the upright, in honour of R. Eliezer; and they are still standing thus inclined. Again he said to them: 'If the *halachah* agrees with me, let it be proved from Heaven!' Whereupon a Heavenly Voice cried out: 'Why do ye dispute with R. Eliezer, seeing that in all matters the *halachah* agrees with him!' But R. Joshua arose and exclaimed: '*It is not in heaven.*'[1] What did he mean by this?—Said R. Jeremiah: That the Torah had already been given at Mount Sinai; we pay no attention to a Heavenly Voice, because Thou hast long since written in the Torah at Mount Sinai, *After the majority must one incline.*[2]

R. Nathan met Elijah[3] and asked him: What did the Holy One, Blessed be He, do in that hour?—He laughed [with joy], he replied, saying, 'My sons have defeated Me, My sons have defeated Me.' It was said: On that day all objects which R. Eliezer had declared clean were brought and burnt in fire.[4] Then they took a vote and excommunicated him.[5] Said they, 'Who shall go and inform him?' 'I will go,' answered R. Akiba, 'lest an unsuitable person go and inform him, and thus destroy the whole world.'[6] What did R. Akiba do? He donned black garments and wrapped himself in black,[7] and sat at a distance of four cubits from him. 'Akiba,' said R. Eliezer to him, 'what has particularly happened

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(1) Deut. XXX, 12. (2) Ex. XXIII, 2; though the story is told in a legendary form, this is a remarkable assertion of the independence of human reasoning. (3) It was believed that Elijah, who had never died, often appeared to the Rabbis. (4) As unclean. (5) Lit., 'blessed him,' a euphemism for excommunication. (6) I.e., commit a great wrong by informing him tactlessly and brutally. (7) As a sign of mourning, which a person under the ban had to observe.

Psalm 115:12-18

The Lord who has remembered us will bless; he will bless the house of Israel; he will bless the house of Aaron; he will bless those who revere the Lord, small and great alike. May the Lord increase you, both you and your children. May you be blessed by the Lord, Creator of heaven and earth. The heaven is the Lord's heaven, but the earth he has given to mankind. The dead cannot praise the Lord, none of those who sink into silence. We will bless the Lord henceforth and forever. Praise the Lord!

On Rosh Ḥodesh and the last six days of Pesaḥ omit:

Psalm 116:1-11

(I love the Lord, for he hears my supplications. Because he has inclined his ear to me, I will call upon him as long as I live. The pangs of death encircled me; the agony of the grave seized me; I was in distress and sorrow. But I called upon the name of the Lord: "O Lord, save my life!" Gracious is the Lord, and righteous; our God is merciful. The Lord protects the simple; when I was brought low, he saved me. Be again at rest, O my soul, for the Lord has dealt kindly with you. Thou hast delivered my soul from death, my eyes from tears and my feet from stumbling. I shall walk before the Lord in the world of life. I trust even when I cry out: "I am greatly afflicted." [I have faith] even when I say in haste: "All men are deceitful.")

Psalm 116:12-19

What can I render to the Lord for all his kind acts toward me? I will take the cup of deliverance, and will call upon the name of the Lord. My vows to the Lord I will pay in the presence of all his people. Grievous in the sight of the Lord is the death of his faithful followers. O Lord, I am indeed thy servant; I am thy servant, the son of thy servant; thou hast removed my chains. To thee I offer thanksgiving, and call upon the name of the Lord. My vows to the Lord I will pay in the presence of all his people, in the courts of the Lord's house, in the midst of Jerusalem. Praise the Lord!

sitions are very subtle.' So he went and sat before him; and on every dictum uttered by R. Joḥanan he observed: 'There is a Baraitha which supports you.' 'Are you as the son of Laḳisha?'[1] he complained: 'when I stated a law, the son of Laḳisha used to raise twenty-four objections, to which I gave twenty-four answers, which consequently led to a fuller comprehension of the law; whilst you say, "A Baraitha has been taught which supports you:" do I not know myself that my dicta are right?' Thus he went on rending his garments and weeping, 'Where are you, O son of Laḳisha, where are you, O son of Laḳisha;' and he cried thus until his mind was turned. Thereupon the Rabbis prayed for him, and he died.

[84*b*] [Reverting to the story of R. Eleazar son of R. Simeon] yet even so,[2] R. Eleazar son of R. Simeon's fears were not allayed,[3] and so he undertook a penance. Every evening they spread sixty sheets for him, and every morning sixty basins of blood and discharge were removed from under him. In the mornings his wife prepared him sixty kinds of pap,[4] which he ate, and then recovered. Yet his wife did not permit him to go to the schoolhouse, lest the Rabbis discomfort him. Every evening he would exhort them,[5] 'Come, my brethren and familiars!' whilst every morning he exclaimed, 'Depart, because ye disturb my studies!' One day his wife, hearing him, cried out, 'You yourself bring them upon you; you have [already] squandered the money of my father's house!'[6] So she left him[7] and returned to her paternal home.[8] Then there came sixty seamen who presented him with sixty slaves, bearing sixty purses.[9] They too prepared sixty kinds of pap for him, which

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(1) The full name of Resh Laḳish was R. Simeon b. Laḳish. Weiss, *Dor*, II, 71 deduces from the use of Laḳisha here that Laḳish was not a patronym but the name of a town, בן or בר meaning 'a citizen of,' i.e., R. Simeon, a townsman of Laḳish. But Bacher, *Ag. der Pal. Am.* I, 340, 1 defends Laḳish as a patronym. (2) Notwithstanding that his fat did not putrefy; v. *supra* 83*b*. (3) Lit., 'his mind was not at rest', that he had not ensnared innocent men too. (4) Made of figs (Rashi). (5) His pains and sores personified. (6) By illness. (7) Lit., 'rebelled'. (8) The Heb. expression means her father's house after his death. (9) These seamen had encountered a violent storm at sea, and had prayed to be delivered for the sake of R. Eleazar son of R. Simeon. This gift then was a thanksgiving offering to him (Tosaf.).

Stamp Corner

Honoring Loschmidt

ALFRED BADER

Alfred Bader,
924 East Juneau Avenue,
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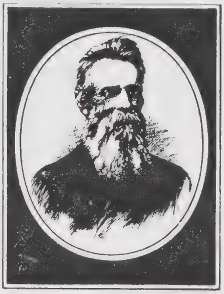
One of the most surprising and instructive stamps honoring chemists in this decade is the Josef Loschmidt stamp (1) issued by Austria in 1995 to commemorate the 100th anniversary of Loschmidt's death on July 8, 1895. In the nineteenth century, Loschmidt was known as an able physicist, the man who first calculated the Loschmidt/Avogadro number in 1865.

In 1861, Loschmidt published a little book [1] (Fig. 1) giving the structural formulas of a great many compounds. Coming from an unknown high school teacher in Vienna, a man without a Ph.D., the book was virtually ignored. It was mentioned only twice in rather derogatory footnotes written by August von Kekulé and in a brief abstract. Not a single Austrian chemist of the nineteenth century ever referred to this book.

Then around 1910, Richard Anschütz, Kekulé's former secretary and his successor as Professor of Organic Chemistry at the University of Bonn, discovered Loschmidt's book, which by then was already very rare. Anschütz was astounded to see that in 1861, the very year in which Kekulé had published his opinion that one could not depict structural formulas, Loschmidt had published several hundred structures, many of them correct and clear. Among these were structures for cyclopropane, mannose, benzene, toluene, phenol, aniline, benzidine, and acetic acid, which was shown on the first-day postmark (2).

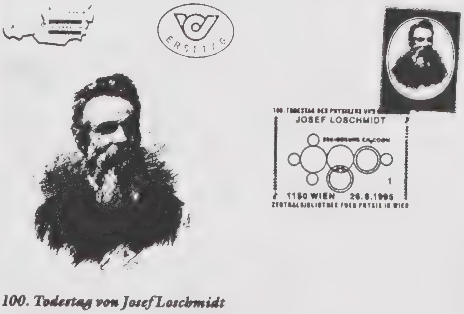
Anschütz published an article on Loschmidt [2] and then went to the enormous trouble of taking Loschmidt's book, reformatting it so that it became very much more readable, and arranging for the publication of the reprint in *Ostwalds Klassiker der exakten Wissenschaften* [3] (Fig. 2).



In 1945, Moritz Kohn [4] published a long article on Loschmidt, essentially abstracting Anschütz's work. Apart from that, few chemists knew anything about Loschmidt's chemistry until William J. Wiswesser of the Wiswesser Line Notation published a startling article [5], "Johann Josef Loschmidt (1821-1895): A Forgotten Genius." The article ended with "all his contemporaries failed to realize that that tiny book of 1861 was really the masterpiece of the century in organic chemistry."

Since then, a good many papers have appeared describing Loschmidt's work as a chemist, and in June 1995, the University of Vienna held a symposium honoring Loschmidt's memory. Among the eminent chemists speaking there were Professor Max Perutz, the Nobel laureate, Professor Carl Djerassi from Stanford, Professor Ernest Eliel from the University of North Carolina, and Professor Albert Eschenmoser from the ETH. The lectures will be published by Plenum Press.

The postage stamp honoring Loschmidt shows beneath his portrait his structure of cinnamic acid. Chemists will note that this was published four years before Kekulé's circular structures of aromatic compounds and long before chemists were certain that the double bond in cinnamic acid is really *trans*. Surprisingly, the stamp does not show Loschmidt's greatest achievement in physics, the Loschmidt number. Unfortunately, at A.S. 20, the value of the stamp is very high, yet it is of such importance that it will surely interest every serious collector of stamps related to chemistry.

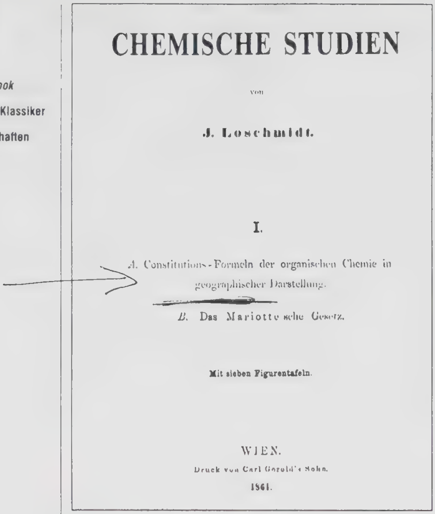


Above: *(1)*

Right: *(2)*

Fig. 1. Title page of Loschmidt's book (Aldrich reprint).

Fig. 2. Loschmidt's book reprinted in Ostwalds Klassiker der exakten Wissenschaften *(Aldrich reprint).*



CHEMISCHE STUDIEN

von

J. Loschmidt.

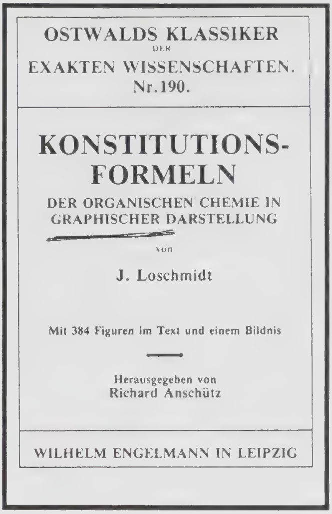
I.

A. Constitutions-Formeln der organischen Chemie in geographischer Darstellung.

B. Das Mariotte'sche Gesetz.

Mit sieben Figurentafeln.

WIEN.
Druck von Carl Gerold's Sohn.
1861.



OSTWALDS KLASSIKER
DER
EXAKTEN WISSENSCHAFTEN.
Nr.190.

KONSTITUTIONS-FORMELN
DER ORGANISCHEN CHEMIE IN GRAPHISCHER DARSTELLUNG

von

J. Loschmidt

Mit 384 Figuren im Text und einem Bildnis

Herausgegeben von
Richard Anschütz

WILHELM ENGELMANN IN LEIPZIG

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3. Anschütz, R. Ed. *Konstitutions-Formeln der organischen Chemie in graphischer Darstellung von J. Loschmidt;* Ostwalds Klassiker der exakten Wissenschaften No. 190; Wilhelm Engelmann: Leipzig, 1913. Reprinted by the Aldrich Chemical Company, Milwaukee, WI Cat. No. Z-18577-9, 1989
4. Kohn, M. *J. Chem. Educ* **1945,** *22,* 381
5. Wiswesser, W. J. *Aldrichimica Acta* **1989,** *22*(1), 17

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202
Phone: 414/277-0730
Fax: 414/277-0709

A Chemist Helping Chemists

January 16, 1997

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

I was in England until January 6th, but Cheryl Weiss faxed me your letter of January 1st regarding the slides required from the Fitzwilliam Museum.

Unfortunately, there have been a great many staff changes at the Fitzwilliam, but one of our best friends, Professor Ralph Raphael, has his office just around the corner from the Fitzwilliam, in the Chemistry Department. Hence, I wrote to him on January 4th, and I enclose a copy of my letter.

I very much hope that you will be receiving the slides .

With all good wishes for 1997, I remain,

Yours sincerely,

AB/cw

Enclosure

To Ralph Raphael

Cornell University

Department of Chemistry
Baker Laboratory
Ithaca, New York 14853-1301 USA

1/1/97

Dear Ms. Weiss:

Let me be presumptuous, since Alfred is probably still in England. Please ask him, on my behalf:

Alfred: Do you have any friends at the Fitzwilliam Museum in Cambridge? You have friends everywhere... If you do, ask them if they could provide me with a color slide(s) of a pair of paintings in their collection — Bartolommeo di Giovanni's "The Story of Joseph". If I use it, of course I'll seek permission.

Happy New Year.

Roald

NAPOLI (Museo Archeologico Nazionale)
Hermes in riposo, bronzo proveniente
da Ercolano.

3/9/96

Dear Alfred,

I don't mean to impose a burden of reading, but since you liked the last chapter here are drafts of two more from the book that consumes me now.

Stupid reviewers thought the art should be removed from "You shall not deviate to the left or to the right — can you imagine that?

It will be resisted

Ronald

522
Ed. Vincenzo Carcavallo - Napoli
Via S. Baldacchini 29 - Tel. (081)204694

Cornell University

Department of Chemistry
Baker Laboratory
Ithaca, New York 14853-1301 USA

September 10, 1996

Dear Friends,

Our colleague Roald Hoffmann will be celebrating his 60th birthday next year, and the Cornell chemistry department is planning to host a symposium in honor of this occasion.

The symposium will be held on Saturday, July 19, 1997 (Roald's birthday is actually on July 18). We plan to have a date of invited talks on a wide variety of topics, reflecting Roald's broad range of interests both scientific and nonscientific, followed by an informal family-style barbeque in the evening. There will also be an informal poster session on Sunday morning for those who wish to make contributed presentations.

Please reserve the date on your calendar. If you would like to be put on the mailing list to receive further information about the symposium in the near future, please notify Greg Ezra (gse1@cornell.edu) or Frank DiSalvo (fjd3@cornell.edu) either by e-mail or letter.

We look forward to hearing from you soon.

Sincerely,

Greg E
Gregory S. Ezra

Francis J DiSalvo
Francis J. DiSalvo

EXCELLENCE
WITHIN

GRADUATE FELLOWSHIPS

The 1995-96
Benefactors and Recipients of
Named Graduate Fellowships at
The Graduate School of Arts and Sciences

The Graduate School of Arts and Sciences
Columbia University
New York, New York

April 1996

This book honors alumni, friends, and organizations who have given their names to the fellowships that support our students -- and the talented men and women who were chosen as the recipients of those fellowships for the 1995-96 academic year.

We applaud these generous benefactors for the active role they play in the life of the School. Their spirit of involvement has sustained and nurtured Columbia's Graduate School over the years, while fostering the ideals of higher education. They have earned our thanks, our gratitude, and our lasting respect.

Eduardo R. Macagno
Dean, Graduate School of Arts and Sciences

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Lorrin T. Brownmiller
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Cornell University

Department of Chemistry
Baker Laboratory
Ithaca, New York 14853-1301 USA

May 4, 1996

Dear Alfred,

I can see that you were as moved as I was by the Rav Soloveitchik analysis of the two Adams (I trust you've seen his book since then). And you have put it to excellent use, as well as the other passage that you cite.

[In that one, Rowland's coworker, who quite appropriately shared the Nobel Prize with him, is Mario Molina. It was my mistake, not yours]
[Also, I don't quite know how to handle this, but my book is coauthored with Shira Leibowitz-Schmidt. It is me that I found the Soloveitchik text and wrote the 2 passages you quoted. So it's OK to cite me alone. But if you publish this, please mention Shira]

All in all, I am a blend of Roald and Ayyal. I'm inconsistent. I'm less worried than you about chemophobia. And I believe deep down in the goodness of people, even those who unthinkingly would shut off the wonders of chemical creation. I believe in opening up a dialogue with them, with all people, by praising the wonders of chemistry yet recognizing its dangers. It's so hard to carve out that middle ground; people only want the extreme position. I keep trying, I think I can do it. And you also through your deep interest and hard work in art are able to cross several worlds.

You know I love to write. So here are some more, mercifully shorter pieces, mostly "educational" in nature.

Be well, friend

+ Amer Scientist
column

Cs_3Te_{22}, The One We Now Know

Roald Hoffmann

I'm supposed to be a theoretical chemist, but really I'm a scavenger of interesting molecules. My pickings are from this flood of scientific journals; Chemical Abstracts says there were 687,789 articles last year that I should have read. Thanks to what used to be the best library in the world, and to my conditioning myself to feeling guilty if I don't look at as many new articles as I can, I glance at 18.56% of them. I look at a molecule, and if I understand it from a theoretical point of view, I go on to the next.

With 35 years experience and lots of molecules in my head, most seem like variations on a theme. I don't disregard them, useful or beautiful as they are. But their geometries fit a pattern. They are not strange; they are friends. I go on to find the one I do not know. Here I tell you of one such encounter.

In a February 1995 issue of Angewandte Chemie (this journal, a close competitor with the Journal of the American Chemical Society for being the best chemistry journal in the world, is also published simultaneously in an English edition) W.S. Sheldrick and M. Wachhold published a paper on the synthesis and structure of Cs_3Te_{22}. Now Te has a profligate chemistry; were there one element that I had to recommend to a solid state chemist to work on, an element that forms a myriad compounds with other elements, almost everyone a puzzle, it would be Te (indium would be a close second). Tellurium, lying under oxygen, sulfur, and selenium, in between antimony and iodine, just has a ball, entering into a great range of weak bonding interactions with itself. Carbon, by comparison, is abstinence itself, forming strong, oh so strong bonds (fortunate for us). With carbon it's yes or no, single bond (or double, or triple) or no bond; for tellurium there is constant flirtation with other tellurium partners, in the range between a bond and no bond.

So... Not only Cs_3Te_{22}, a weird stoichiometry that we wouldn't dare to show our beginning students (what's the oxidation state of Te?), but some nine other compounds (phases, as they are called in the trade) were known at the time of the Sheldrick and Wachhold paper. These ranged from tellurium-rich $CsTe_5$ to cesium–rich Cs_3Te_2. Two more have been made since.

These compounds are not discrete molecules, weakly held together in a molecular crystal. They are extended structures, in which networks of atoms, bonded in part by covalent, in part by ionic forces, march in orderly fashion through the crystal. But I've been withholding the structure too long — Illustration 1 shows it in a perspective view (cesiums are dark, telluriums light).

Illustration 1 here

The first feature one discerns is crown-shaped eight-membered rings of tellurium atoms. Two such rings cluster around a Cs, forming a cubical environment for the alkali atom. I look at this, searching for similarity and difference. As do the synthesizers of the

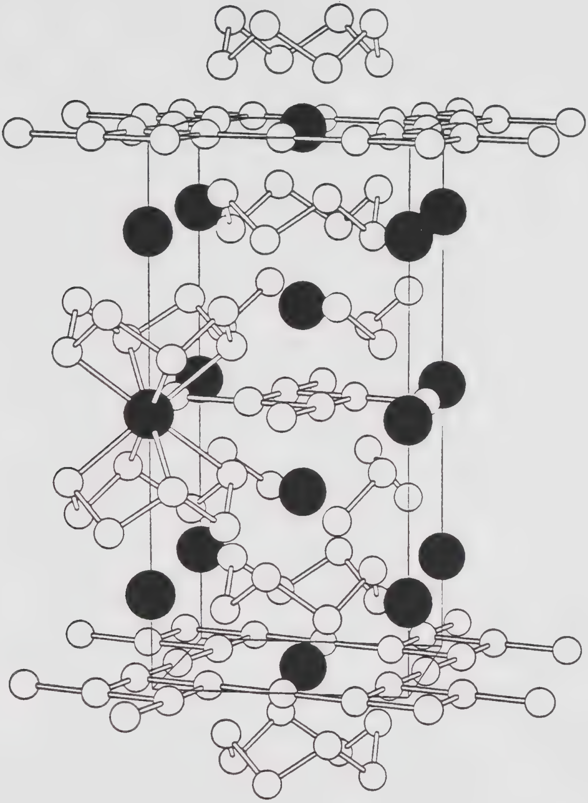

Illustration 1: The structure of Cs_3Te_{22}, with one unit cell outlined. Small open circles are Te atoms, while Cs atoms are marked black. There are a few Te_2 grouping scattered, but these are truncated fragments of Te_8 rings.

molecule, who know just as many structures as I do.

And I remember that sulfur, for which a host of allotropes is known (now there is an interesting story, that of the sixteen sulfurs of Erämetsä) readily forms such eight-sulfur crowns. And so does selenium. That's similarity, á la Mendeleyev. But, for tellurium such a ring had never been seen! A surprise but not a surprise; still, what a weird thing — to have to make a tellurium compound to find in it a geometry that elemental tellurium should show. This is the fun of chemistry, and why the field gets along with a smallish number of theoreticians. Who could have predicted Te_8 rings in Cs_3Te_{22}?

And noone predicted the other piece of the structure, an incredible planar $CsTe_6$ sublattice, which you can see "side-on" in Illustration 1, and which is shown "end-on" in Illustration 2. To get to the $CsTe_6$ formula, you can look at the "unit cell"(the repeating unit of the net), drawn as a box in the Illustration, and count up the atoms in it.

Illustration 2 here

If you like symmetry, this neat structure is for you. This is a rare two-dimensional net; yes, Escher has drawn it, and I think it is in the Alhambra. But I had not seen it in any molecule. The only symmetry elements of this net are four-fold and two-fold rotational axes.

Now some electron counting: Since the cesiums are prone to give up their one valence electron each and bond ionically in this solid (and the Cs-Te distances are consistent with this), and the two Te_8 rings per Cs_3Te_{22} formula are happy as neutral, elemental Te_8, the only place to go for the three electrons that the cesiums give up is into

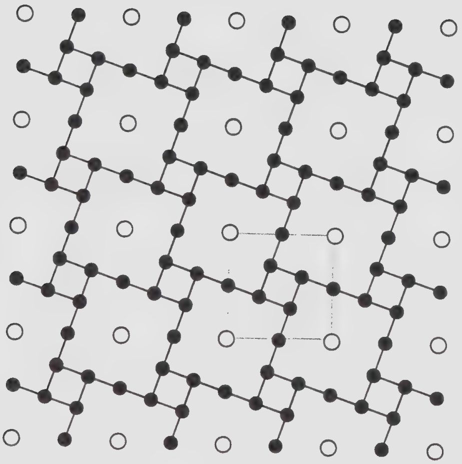

Illustration 2: The $CsTe_6$ net in Cs_3Te_{22}. One unit cell is outlined.

that Te_6 net. To put it another way $Cs_3Te_{22} = (Cs^+)_3(Te_8)_2\,Te_6^{3-}$.

Once I'm through admiring the symmetry of the Te_6 net, I look at its structural features, to see if I understand them. There are squares of Te — aha, I remember John Corbett and his coworkers made Te_4 squares nearly a quarter of a century ago (and there has been work by Gillespie's group on the corresponding Se analogues). But Corbett's compounds were isolated molecules, each Te two-coordinate, and they carried a 2^+ charge overall. The Te's in the squares in the Sheldrick and Wachhold compound are three-coordinate, and negatively charged. And the coordination geometry is weird — not trigonal or trigonal pyramidal (all Te-Te-Te angles equal, 120° or less) but what we can loosely call T-shaped.

Per Te_6 unit there are four such T-shaped atoms. Connecting these are two-coordinate telluriums. That seems as it should be — tellurium's normality is expressed by forming two bonds, except... the usual Te-Te-Te angle in those normal tellurium compounds (the analogues of water, alcohols or ethers) are near 90°. In the Te_6 net in Cs_3Te_{22} these angles are 180°.

This is where I wake up, as did my coworkers Qiang Liu, from China, and Norman Goldberg, from Germany. Not that we needed waking up, for noone had seen such a net before. But now that we realized how strange the seemingly innocent geometries of the net components were, we knew we had to understand this molecule. Having the tools in hand, we tried.

Our theoretical story will appear around the time you read this. In part it is a computational tale — we specialize in the kind of approximate solutions to

Schrödinger's equation to which all other computations are superior. And we bootstrap ourselves out of the lowest reaches of quality of computation by constructing portable explanations, based on molecular orbital arguments. We read the clues in this structure: T-shaped telluriums(that reminds us of BrF_3, also T-shaped), linearity where bending would have been expected (that reminds us of linear I_3^- and XeF_2), and electron richness (Te_6^{3-}). All of these features, geometrical and electronic, point to what chemists sometimes call hypervalence, and also to a framework of ideas under the rubric of 'electron-rich three-center bonding". There was a surprise, in that these compounds didn't quite fit these non-classical extensions of normal bonding — they were not classically non-classical!

For the rest of the story you will have to read our paper. We understand the bonding in the end, or at least tell a good story about it. We predict some further structures, and incredibly one of these has been made. But the theory is in some ways unimportant here, for we were followers and rationalizers. What is important is that the molecule has been made, in its dazzling interest.

The next time I see that net, in another compound, it will be—to me—just a little bit less interesting. That's fine; another issue of Angewandte Chemie is on its way.

P YO

Pimentel Award address
J. Chem. Educ. eventually

TEACH TO SEARCH

Roald Hoffmann

Department of Chemistry, Cornell University, Ithaca, NY 14853

George Pimentel was a wonderful man, whose heart and soul were in chemistry. And just as much in research, in which he excelled, as in teaching. From his writing it is clear that he did not separate the two. Nor do I, which is why I am happy and proud to be associated both with an award given in George Pimentel's name, and especially one in chemical education.

I will speak of two themes, with digressions:

(1) The inseparability of teaching and research. Or, for that matter, of chemistry and the world.

(2) The necessity of chemists to teach broadly, to speak to the general public. I will comment on the means to do so, and the tensions that arise in the process.

But before I launch into these subjects, let me say some words about how I feel about teaching and receiving this award.

Whatever success I have I owe to teaching. The logic or rhetoric of teaching underlies my research within chemistry, and my writing outside of chemistry. As I began to think about this, I felt suddenly a little less guilty about receiving an award in chemical education.

Let me tell you why I felt, feel guilty: What am I -- viewed by the community of chemistry as a researcher whose work has received ample recognition -- doing getting an award that should be given to those who have dedicated their lives to chemical education, who have toiled so hard? When there aren't too many of these awards around...

A second source of guilt for me is that I suspect that a significant component in the thinking of the Pimentel award committee was my role in making the Annenberg/CPB television course in chemistry, "The World of Chemistry". I was a member of the team, indeed, and my soul and sweat went into the project. But the part I played — more than just being a pretty face, true — was in fact much, much smaller than those of several other people, who really deserve the recognition.

I will tell you about those people in time. I do feel guilty about receiving this award, but my guilt is assuaged, just a little, by pride in the fact that I have taught thousands, and I have taught others to teach, that I have taught, subtly, the research community in chemistry that teaching strategies in research are productive, and that I have contributed, I think, to the growing respect for teaching (in the broadest sense, not only in the classroom) in the community of chemistry.

Let me address first the issue of teaching and research: A damaging misconception about modern universities is that research dominates and diminishes teaching. And that the tension of balancing (unsymmetrically) the twain is unhealthy. Defenders of the universities argue that the two functions are complementary, and that research or scholarship enhances the quality of teaching. I go further: I say research and teaching are, quite literally, inseparable. And that a measure of tension is essential for creation.

A root of the error, I believe, is thinking of learning in terms of place rather than audience. Places (classrooms, labs, library carrels) are, indeed, circumscribed. But the audiences of learning (undergraduates, graduate students, faculty, our minds) always shift, overlap and enrich each other, like the colored glass bits of a kaleidoscope.

As I reflect on the possibility of a separation of research and teaching, I look at my research group. We meet twice a week -- four graduate students, four postdoctoral associates and I. One time we talk about the incredible, fertile literature of chemistry, while in the other session one of the people in the group reports on her work in progress. We also ask why marzipan pigs are popular in Denmark, explain to our foreign group members all those football and baseball metaphors in colloquial English, and try to guess who is likely to be the author of those scurrilous referee's comments on our last paper. In these group meetings half the time I'm giving a monologue, the rest of the time the hardly shy rest of this research family speaks. Is that research, is that teaching?

I travel to the University of British Columbia to lecture about my work, about making and breaking bonds in the solid state. 90% of the audience consists of graduate students, with a sprinkling of undergraduates. I talk to <u>them</u>. Is that research, is that teaching? I think the answer in both cases is yes. It's research and it's teaching.

These two poles of our university experience are inseparable. They permeate each other. The struggle to do both well enriches our personal intellectual lives, and enhances our contributions to society.

I am certain that I have become a better researcher, a better theoretical chemist, because I've had to teach undergraduates. When I began at Cornell, for instance, I thought I knew all about thermodynamics, all those beautiful partial differential equations that related the derivative of A with respect to B to C. But thermodynamics is a subject of great richness, with practical, common sense roots (steam engines, the boring of cannon) and a mathematical structure of breathtaking sophistication. I had only followed the latter, and hadn't really understood the full empirical beauty of "thermo" until ...I had to explain the subject to students without the crutch of the mathematical apparatus. The more I taught beginning classes, the more important it became to me to explain. The rhetoric of pedagogy permeated my research. I think those in the community of chemistry who know my work will recognize what I mean.

I think there is nothing specific to me in all this. I believe that rather than treat research and teaching as disparate activities, it is more productive to cast the discussion in terms of audiences for creative work in science or the humanities.

In the beginning is research or discovery, a gleam of the truth, or of a connection, within an individual's mind. Actually I've experienced such moments, and so have others, most often not in isolation, but in discourse with another person. Or when I sit down to write a paper, before me the draft or progress report by one of my students.

In fact understanding already formed in the inner dialogue between parts of me, me and an imagined ideal audience of one, or of a multitude, in the lonely dialogue with the voices of skepticism and self-doubt that are all me, all of me.

Deep in
it's a docile crowd
most of the time, lazing
around, waiting for the train
of concentration to haul a few words
onto paper. It listens, then it stirs, the one
that speaks in many voices, to say:
these are just words, falling limp
into the untensed space they need sculpt, or:
make me understand.
They hate my compromises.
Here and there they offer up a phrase.
In their babble I hear the voices

of my teachers rise from a page or café. Sometimes
one speaks with an accent -- I think
it's my father, it's him, the world
I have to please.
For them I leave no word unturned.
For it I sing, tone-deaf that I am,
the song that frees itself within.

In the next stage the audience expands to my research group. In the process of talking to them the depth of my understanding of the discovery deepens, takes a stronger hold on reality. Then I write a technical paper. Now my audience is out of my control. Writing is the message that abandons, as Jacques Derrida has called it. I can't grab that removed reader in Poznan or Puna and tell him, no, you must read it that way, and not this way. It has to be all there, in the words with which I struggle. It has to be there -- the substance of what I found, and the argument to convince him or her, the absent reader. And I write for that audience from a position of substantive ignorance about them -- I don't know their preparation, their level of sophistication, their willingness to work to reach enlightenment! It begins to sound an awful lot like teaching.

The writing of a research paper to me is in no way an activity divorced from the process of discovery itself. I have inklings of ideas, half-baked stories, a hint that an observation is relevant. But almost never do I get to a satisfactory explanation until I have to, which is when I write a paper. Then things come together, or maybe I make them come together. F. L. Holmes has argued convincingly the same point, that scientific writing and scientific discovery are not disparate activities. In an analysis of draft manuscripts of a Lavoisier memoir on respiration he "...could watch important ideas emerging, growing, changing form or decaying during the evolution of a scientific paper."

A technical seminar at another university introduces another audience. Sure, I want to impress my colleagues, claim precedence, power, please real or constructed parents. Many things go on subliminally in the course of any talk. Yet most of all I want to impart real, significant new knowledge. But the audience includes people of disparate backgrounds. The organic chemists may not know much about my present loves, which are surface and solid state chemistry. Depending on their background, different parts of the audience may attach different meanings to the plain English words at my disposal. There are many graduate students here. I want to teach all, convince all. Remarkably, incredibly, we can do it, speak to many audiences at the same time. That's what teaching is all about.

To me, the steps from a research seminar to teaching a graduate course, then an undergraduate one, are small moves in interacting with the continuous, overlapping spectrum of audiences. In the theater of the mind the audience is always shifting, never constant. There are different strategies, call them tricks, the stuff of experience, that one applies with these audiences of young people and that one might not try in a research group meeting. But the similarities of pedagogical strategy across the spectrum of teaching/research far exceed the differences.

The spiritual rewards for opening a person's mind, sharing newfound knowledge, are also quite similar. I've taught introductory chemistry many times, to thousands of students. There is the same unmitigated pleasure that hits me when I detect, on an examination or by the nonverbal signs students give in lectures, that someone has understood the magnificent and simple logic of the mole, so that he or she can tell me how much sulfur there is in a pound of sulfuric acid.

To return to my main point, I wish to argue that the desire to teach others, enhanced by being <u>obliged</u> to teach others, leads to greater creativity in research. The rhetorical imperative operates to make a scientist or scholar examine widely the potential responses (objections?) of his or her audience. Having to teach enlarges one's encounters with real audiences, therefore sharpens the imagined audience one engages in the inner dialogue in the course of research.

As my friend R. Freis has pointed out, following St. Thomas Aquinas, teaching is truly a cooperative art. It works together with the nature of the student as learner, knower, apprentice, in order to bring that nature to its perfection. Teaching is clearly also a rhetorical act. But it is more than mere persuasion, because of the empathetic, reflexive aspect of it being cooperative. How could the mind that faces up to the problem of teaching a novice something new and difficult possibly avoid using the same strategies in explaining to itself something still more new, more difficult? Which is what people call research.

2

I want to try to illustrate to you what I mean by the rhetoric of teaching influencing my research style. To do that I've picked a recent paper, entitled "A 2,3-Connected Tellurium Net and the Cs_3Te_{22} Phase", written by Qiang Liu, Norman Goldberg, and myself, to be published soon in Chemistry, A European Journal.

Our work grew out of a paper we saw by Sheldrick and Wachhold in a February 1995 issue of Angewandte Chemie (W. S. Sheldrick; M. Wachhold, Angew. Chem. Int. Ed. Engl. 1995, 34, 450), who reported a new Cs_3Te_{22} compound. Now the chemistry of tellurium is very rich; for instance in the Cs-Te system some nine binary cesium telluride phases ($CsTe_4$, $CsTe_5$, Cs_2Te, Cs_2Te_2, Cs_2Te_3, Cs_2Te_5, Cs_3Te_2, Cs_5Te_3 and Cs_5Te_4) had been reported earlier, and two more have been made since.

The beautiful structure of the Sheldrick and Wachhold compound (Figure 1) displays a number of unusual features. Discrete crown Te_8 entities can be easily identified in Figure 1. Though such eight-membered crown-shaped molecules are well known for sulfur and selenium, they had not been previously observed for tellurium. Also apparent are infinite two-dimensional sheets that are formed by Te atoms and which include one Cs atom per six telluriums. Each Cs atom in the $CsTe_6$ sheet is located in the center of a large square of 12 Te atoms.

The structure may also be described as consisting of two different types of layers: $CsTe_6$ sheets separated by layers of $CsTe_8$ crowns: $[CsTe_8]_2[CsTe_6]$. If one assumes the Te_8 rings to be neutral molecular entities and assigns the valence electrons of cesium fully to the only atoms left, the tellurium sheets, the compound may be described as $[Cs^+]_3[Te_8]_2[Te_6{}^{3-}]$. The $Te_6{}^{3-}$ net is definitely electron-rich.

Figure 1 here

The pattern of the $CsTe_6$ sheet (Figure 2, looking down the c-axis onto the sheet; the darker and larger spheres are Cs, the light ones Te) is remarkable. This is a rare net; the C_4 axis is the principal symmetry element present (aside from two-fold rotation axes and the mirror plane containing the sheet itself).

Figure 2 here

So far, you see an intriguing structure; that was apparent to the authors and readers of the initial report -- they saw the same beautiful structure that I show you. And we, as theoreticians, next did the stuff of our trade, a calculation of the electronic structure of the three-dimensional material. The outcome is shown in Fig. 3; it is a so-called band structure, showing the energy levels of the molecule.

Figure 3 here

Now if the pedagogical imperative were not important for me and my group, I think I would have (in an alternative universe, I can't imagine doing so here) stopped pretty much with an analysis of the bonding here; perhaps worried about stability, and reached the conclusion that the material might be a conductor.

But now in my real world -- of trying to understand this big molecule -- of trying to see its connection to everything else in the molecular world, that band structure is just the beginning. I look at that incredible net with four-fold symmetry, and I see in it two kinds of Te atoms. One is linear, bonded to two other Te atoms. Call this Te2. The other, which we call Te3, is T-shaped,

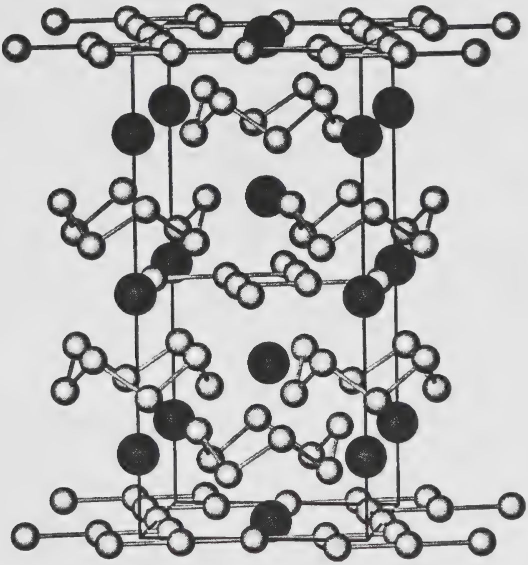

Figure 1 The structure of Cs_3Te_{22}. Small circles are Te atoms, the large gray circles are the Cs atoms.

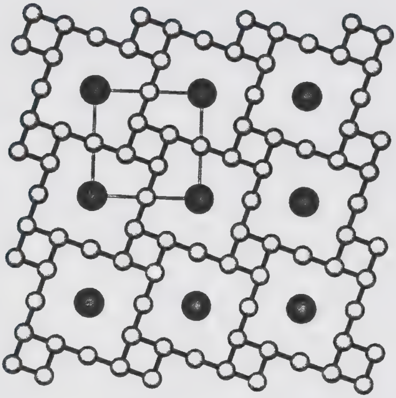

Figure 2 A top view of the $CsTe_6^{2-}$ net. One unit cell is highlighted by a square.

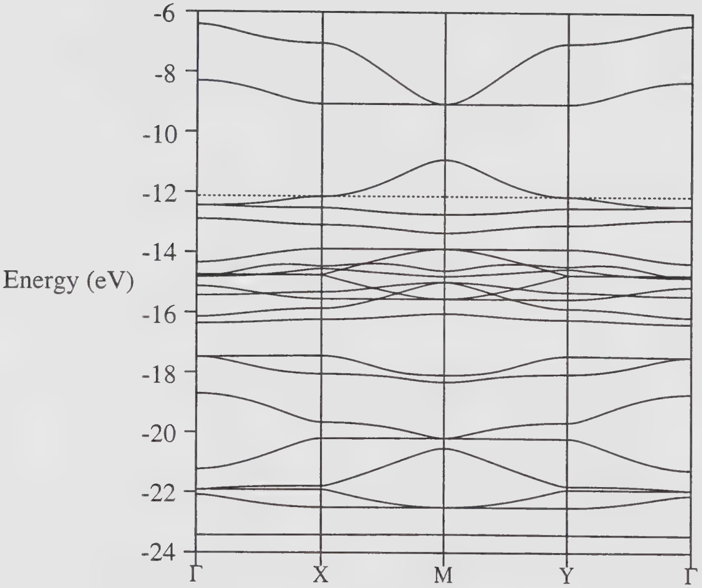

Figure 3 Band structure for the Te_6^{3-} sheet.

bonded to three Te atoms. It is important to note here that the Te2 and Te3 notation does not refer to a crystallographic numbering; it is our way of reminding ourselves of the coordination environment of each Te.

I think about these; where else have I seen two- and three-coordinate tellurium or its analogues? Where else have I seen tellurium squares?

Well, for two-coordinated main-group EX_2 molecules both bent (H_2O, H_2Se, H_2Te, and Te_3^{2-}) and linear configurations (XeF_2 and I_3^-) are possible. Why is Te2 linear in this sheet?

The T shape of Te3 reminds one of the BrF_3 molecule, and it does occur in a number of other extended tellurium structures.

As far as squares go, there aren't that many main group element squares around. E_4^{2+} species (E = S, Se, Te) are known, as is Bi_4^{2-}, and they are isoelectronic with electronically happy $C_4H_4^{2-}$. To my knowledge there are no square hypervalent molecular groupings with halogens, noble gases, or metals.

As we wrote this paper, I felt it essential to construct our understanding of the extended structure through molecular models and bonding schemes drawn from model molecules. Which is what we did. We began by looking at a simplified model for Te2 by calculating a Walsh diagram (i.e. how the energy levels of this triatomic varied with bending at tellurium) for H_2Te^{n-}. We found (not surprisingly) that the preferred geometrical configuration of H_2Te^{n-} depends strongly on its electron count. The molecule prefers a bent geometry when it is neutral, as expected. And the triatomic is linear for H_2Te^{2-}, analogous to a hypervalent H_2Xe or F_2Xe. We also looked at a more realistic model for the atomic environment of Te2 in the solid, Te_3^{n-}.

Next I will actually quote a piece of our paper (omitting references, of which there were many), not because it is important, but because it helps me make two points:

> A connection needs to be made here to the classical and well-characterized linear triiodide I_3^-. This species is, of course, isoelectronic to Te_3^{4-}, as is the related XeF_2. The bonding in I_3^- or XeF_2 is very well understood — we have in these molecules an electron-rich three-center bond. If one omits the s orbital on the central atom from the bonding, one expects the level pattern at left in Figure 4, while if the s orbital is included we get the pattern at right. Note in either case that one and only one I-I-I antibonding orbital remains unfilled...

Figure 4 here

Why do I quote this? First, actually the subject just happens to be related to work that George Pimentel did. He and Rundle first explained qualitatively the bonding in triiodide anion and related electron-rich compounds.

Second, I see this section as an example of the teaching imperative influencing research. In this section, and in the paper as a whole, I am intent on drawing the connection to electron-rich three-center bonding. And I will not assume that everyone has seen it. So I repeat an orbital level scheme -- that's part of my teaching in research strategy. Even if that level scheme has been in the literature before. I repeat it because it is part of the story, and the story is incomplete without it, and I am anxious to get into the mind of the poor graduate student assigned by his professor to talk about this paper at the next group meeting, and I'm interested in teaching that graduate student, and -- you know, it actually helps me understand this bonding if I explain it in detail, as if I were teaching...

You can be sure that such pedagogically-driven research strategies are as disliked by some reviewers and some journal editors as they are appreciated by the young researchers who read these papers. Sometimes it has not been easy to get such teaching/research narratives published. But I persevere, and sneak them in.

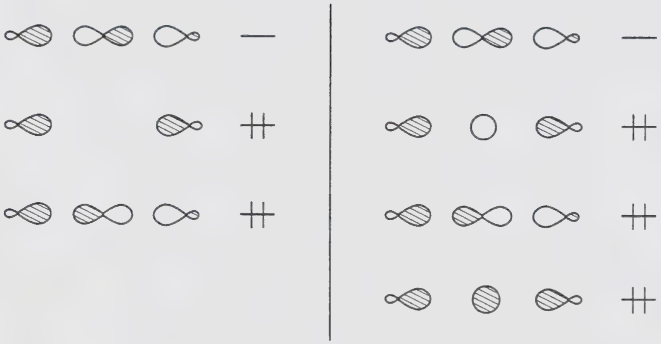

Figure 4 The orbitals involved in the three-center bonding in Te_3^{4-}, I_3^- and XeF_2.

Let me show you another piece of this paper which makes some reviewers see red:

> The T shape reminds one of the BrF_3 molecule, whose bonding is described qualitatively in Figure 5. Note the formal F^- nature of the "axial" fluorines. We see two lone pairs on the Br, a "normal" equatorial Br-F bond, and electron-rich three-center F-Br-F axial bonding. BrF_3 is clearly related to SF_4 and XeF_2. A tellurium analogue (Figure 5 at right) would be Te_4^{4-}...

Figure 5 here

> Let's look at the structure at hand in still another way. Each Te2, linear, is hypervalent, and (if it were maximally hypervalent) could be assigned an electronic structure such as that shown in in Figure 6, left, and a formal charge of -2. Each Te3 can be assigned a locally hypervalent structure, Figure 6 right, and a -1 formal charge. With these charges throughout the net we would have a charge per formula unit, $(Te3)_4(Te2)_2$, of -8. However, the actual charge is only -3! In other words, our Te_6^{3-} net is hypervalent (as the T-shaped Te3 and linear Te2 indicate), but it is not "maximally hypervalent" in the sense of as many electrons as these hypervalent geometries would allow. It is this intermediate reduction stage that makes the electronic structure of Te_6^{3-} truly non-classical and requires a delocalized bonding description...

Figure 6 here

There is much more in this paper, a discussion of an alternative structure (see Fig. 7), of possible fragmentations of the net, and the suggestion on the basis of the computed electronic structure, of two unknown compounds, $[CsTe_6]^-[CsTe_8]^+$ or $CsTe_7$ and $[CsTe_6]^{3-}[CsTe_8]_3^{3+}$ or Cs_2Te_{15}. Both should have structures similar to that of Cs_3Te_{22}, but composed of layers of $CsTe_6$ sheets and

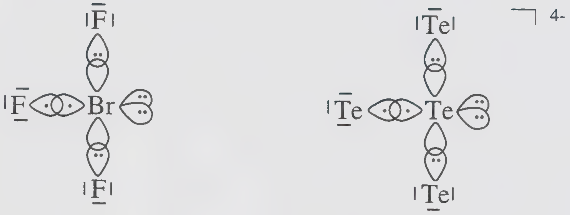

Figure 5 The hypervalent BrF_3 and Te_4^{4-} molecules.

$CsTe_8$ units in 1:1 and 1:3 ratios, respectively. The $CsTe_7$ phase should be metallic. Incredibly, one of these compounds has been made, and it almost (not quite) has the simple structure we predicted.

Figure 7 here

Now I must reign in my enthusiasm for this wonderful molecule, and return to the subject of this lecture. I do hope that by this example I have illustrated what I mean when I say that the rhetoric of teaching has influenced my research. And I want to have enticed you to look at tellurium's weird and fascinating chemistry.

3

Now I turn to what I see as the reasons for talking about science to the public, and the difficulties of doing so. I do not mean to exclude personal and structural reasons -- by these I mean the sheer fun of the study of matter and its transformations, the fact that most of us are employed to teach chemistry, with attendant obligations, and that we do need to train professional chemists. These things we understand well -- they may be fun or a chore, but they are intrinsic to our profession. I want to address in a more general, reflective way, the reasons why we must teach in the broadest possible way, to speak to the public.

(1) There is public and political concern about money spent on science. The public ultimately supports our research through its tax dollars. The informed citizen will let the talented expert carry out his or her basic research. He will accept even that technological benefit is not to be expected. Such a citizen will accept even a measure of vagueness about what is done, and will take the excitement of the scientist as a sign of creative activity. For a while. But at some point we have to tell people (not the least of among them being our parents and spouses) what it is that lures us back to work nights and Sundays, why it's thrilling to open a new issue of the Journal of the American Chemical Society.

(2) Chemophobia is rampant, there is a negative image of chemistry and

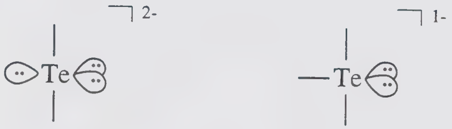

Figure 6 Maximal hypervalence in the Te_6 net would lead to a 2- charge on the linear telluriums (left) and a 1- charge on the T-shaped telluriums (right).

chemists, as the producers of the unnatural, the toxic. This is undeniably true. But at the same time, every survey shows that the public views scientists with high regard and trusts them. This is not irrationality, just nice human inconsistence. People are not machines -- they can both value and be afraid of something, at the same time. But certainly the more people know (of substances, of molecules) the less likely they are to be afraid of what we create.

(3) If we do not know the basic workings of the world around us, especially those components that human beings themselves have added to the world, then we become alienated. Alienation, due to lack of knowledge, is impoverishing. It makes us feel impotent, unable to act. Not understanding the world, we may invent mysteries, new Gods, much as people did around lightning and eclipses, around St. Elmo's fire and volcanic sulfur emissions a long time ago. I feel the growth of antirational movements (and religion is most certainly not one of these), in the form of cults, of interest in the occult and astrology -- these are a modern-day reaction to the mysteries that now science has surrounded human beings with.

(4) My last point of concern about chemical illiteracy and teaching chemistry concerns democracy. Ignorance of chemistry poses a barrier to the democratic process. I believe deeply that "ordinary people" must be empowered to make decisions, on genetic engineering, waste disposal sites, on dangerous and safe factories, or which addictive drugs should or should not be controlled. They can call on experts to explain the advantages and disadvantages, the options, benefits and risks. But experts do not have the mandate; the people and their representatives do. The people have also a responsibility -- they need to learn enough chemistry to be able to resist the seductive words of, yes, chemical experts who can be assembled to support any nefarious activity you please.

Of course there are many audiences for what we want to say:

(A) The children and young people in our schools,
    (i) who will be citizens and not scientists (99%),
    (ii) who might be scientists; who may be motivated to become such

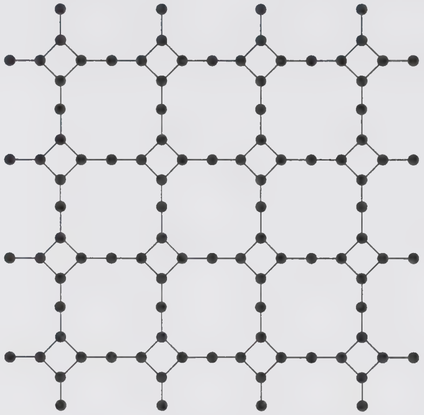

Figure 7 A possible distortion of the tellurium net to a hypothetical D_{4h} Te_6^{3-} sheet.

by what we teach,

(iii) the small unknown subset who will decide the future of the country and of science.

(B) Not children, but

(1) the proverbial general public, let us say those who watch soap operas religiously, and whose labors move the country on,

(2) the politicians and authorities: and I don't necessarily have a bad view of them. I respect the compromises they must make and that I can avoid,

(3) the merchants and business men who power our economy,

(4) our friends in the arts and humanities and religion, the shapers of the spirit, and

(5) other scientists.

It seems that each audience needs a very different approach. And it seems an impossible task to speak to all. But please don't despair. Every teacher has the experience that as impossible as it seems, it is possible to speak to several audiences at the same time.

What are the problems we face in teaching science? What are the attitudes which our students and peoplebring to our subject? Let me describe some, a caricature to be sure:

(1) Science is complicated, too difficult for a normal person to understand. Science is for smart people.

(2) Science doesn't concern me. It's not going to determine if Syracuse does or does not (it didn't) win the NCAA championship, or whether I can buy my beer (or VCR).

(3) Science is boring; it is definitely not fun.

(4) Science is done by rich people, by old European white men with beards.

(5) Science is for people who don't want to talk to other

people but play with computers or things.
(6) Science creates the unnatural, the dangerous.
(7) Science kills the lovely hawk circling the sky and dissects him. Science is unpoetic, inhumane.

These are caricatures and extremes. But I think you recognize them, don't you?

One can attempt to counter these attitudes, one by one. But I would rather make some observations which point to an approach, rather than a specific strategy.

(A) These are perceptions about science (mostly wrong), not realistic assessments. That's OK, we live by ideas and things of the spirit as much as we do by matter. Please accept the strength (and even sincerity) of a perception even when it is at some level wrong.

(B) What we do not understand, we usually find uninteresting and sometimes are just afraid of. What we understand, we may find interesting and may (not always) be unafraid of. This applies to art as well as science — think of attitudes to Stravinsky's music of the beginning of the century. And this is why we must teach, in a myriad ways.

(C) People like facts, but really they love a good story, well told. There is an art to telling stories, and telling stories is very, very old. Stories are human, they are about perceptions, through them a shared understanding forms.

So I think that one way into people's hearts and minds is to tell stories of science. In school it may be done in the midst of a logical development of a subject. To a general audience it's a way to normalize, humanize science and build a piece of understanding. I urge you to explore the power of a story well-told in your teaching.

4

I return to the making of our videocourse, The World of Chemistry.

The course was conceived by Isidore Adler of the University of Maryland and Nava Ben-Zvi of the Hebrew University of Jerusalem. A decade ago they approached the Annenberg/CPB project, who eventually funded the major part of this course. Adler and Ben-Zvi, together with University of Maryland physical chemist Gilbert Castellan, Margot Schumm of Montgomery College and Mary Elizabeth Key, then of St. Albans School in Washington, formed the 'academic team' that conceived the content and supervised the production of the programs. Richard Thomas was the imaginative executive director and producer of the series, working together with the able technical staff at the Educational Film Center, Annandale,Virginia, an Emmy-Award-winning production company. This award is for them as well.

The World of Chemistry is intended for a junior college, four year college, or remote learner audience. It can serve as a complete course in chemistry, but it can also be used as a supplement for courses at any level, secondary school or university, as a resource for young people or industrial workers, or just as entertaining viewing for the citizen at large.

Each program contains the following components:(a) two chemists who appear in nearly all the segments: I, as the presenter or series host, and Don Showalter of the University of Wisconsin at Stevens Point. He has all the fun, since he gets to do the spectacular demonstrations. There are also (b) one or two lively interviews in each segment, (c) some computer animation (no blackboard!), and (d) weaving it all together, over fast-moving montages and footage illustrating the concepts taught, a narration.

Some of the programs teach very directly -- so one of the 26 is on 'The Mole', and two on 'The Driving Forces' and 'Molecules in Action', which explain on the macroscopic and microscopic levels why chemical reactions occur. Other programs describe important chemistries -- those of color, of metals, and of reactions on surfaces. There is a whole program devoted to 'The Chemistry of the Environment'.

In professional television, which is what these programs are, you get what you pay for, to a certain extent. These programs were produced at a per minute cost a half of that of a typical U.S. 'Nova' program, or only one tenth of that of 'Cosmos'. So whereas my friend and colleague Carl Sagan stood in front of the ruins of the library of Alexandria in Egypt, I got sent as far from Washington. DC as Baltimore, Maryland to stand on a wintry day on a tank car of sulfuric acid! Actually you'll see more in these programs than one might have judged from their cost -- they were made with the dedication, sweat and mental energy, mostly unpaid, of a remarkable team of people.

One observation which I would make is that what started out as a weak point of the production turns out to be one of its great strengths. We did not have the money to shoot 10 to 15 minutes of each half-hour from scratch, i.e. illustrating through our own filming the concepts that we wanted to teach. So, we made do with skillfully edited 'stock footage'. This is a euphemism for free or inexpensive film clips obtained from government or industrial sources. An industrial public relations consultant could often identify the source of a scene from the five seconds it is on the screen.

Now this stock footage was, is a weakness; it isn't what we would have done in that ideal, unlimited-budget world of which every film maker dreams. But by being forced to use (fairly, without commercialization) scenes supplied by others, especially by industrial sources, our programs acquired a 'real world' feel to them. I can put it another way: in how many chemistry courses in the world does the instructor show students five minutes of steelmaking, and three minutes of the Hall process? We do, and the visual impact is tremendous.

I want to make some observations on the tensions I see arising in the use of television to teach.

(1) First, a philosophical question: can one teach via television? Or does a switch go on in our minds that this is entertainment?

(2) The process is incredibly expensive. So much of one’s time is spent in

fundraising. But this is typical in the arts, and so it is in science. My friends Ivan Legg and the late Paul Gassman worked very hard on raising the funds to a sequel to The World of Chemistry. We failed. The industrial community, our own industry, was not supportive of our efforts.

(3) The television medium is inherently journalistic. As such it leads to excessive mythologizing -- of individuals, and of the way things happened. This hurts.

(5) There is a continuous treachery of simplification, of making little compromises. In the end it doesn't leave the person making those compromises (me, and maybe I was too sensitive) feeling good about either himself or the process.

(6) The power of images is incredible. Let me tell you a story, which I've written about in Chemistry Imagined:

In the making of a program about the atom, a piece of stock footage that came our way was from IBM. It was about Scanning Tunneling Microscopy (STM), a marvelous technique for imaging surfaces, invented in 1982 by Gerd Binnig and Heinrich Rohrer at IBM's Zurich Research Laboratories. The technique is appealingly simple, and the images it produces so revealing that the invention was immediately recognized as of value, and rewarded by the 1986 Nobel Prize, only three years after the work was published.

The IBM propaganda, justifiably proud, turned on the hype. Now, for the first time, one could see atoms. Their tape showed a striking, false-color "fly-by" across the surface of a silicon crystal.

To the production team for our television show, daunted by the unenviable task of depicting something as intangible as the atom, the IBM footage was a godsend. They made it the centerpiece of a sequence that began with the incredibly beautiful footage of an earthrise on the moon, filmed by the Apollo astronauts, evoking the importance of the moon landing——a voyage, a search, discovery. All the directors' skill, a skill I greatly admired, shaped implicit and overt connections to the STM images. The struggle to form an atomic theory, from Democritus to Dalton, culminated in those appealing pictures of the silicon surface. Now, after such a long time waiting, now we could see atoms.

I nearly went through the roof (which was high up——we were filming in the New York Hall of Science, a structure remaining from the last New York World's Fair). What treason here to 180 years of theory and experiment that through tedious, indirect evidence built a framework of incontrovertible reality for atoms and molecules! That wondrous scanning tunneling microscope would never have been built, were it not for that painfully won, indirect but certain knowledge that atoms combine into molecules and extended arrays with precise, known geometries.

The directors ignored my concern——just another scientist adding qualifications to what anyone could see. But there was a slot, a minute long, which I was given to close the program. For that I wrote the script myself. I quickly substituted the following:

> We've looked in this program at the structure of the atom. We've described the experimental and theoretical steps leading to our modern picture of the atom, this electron cloud around a nucleus. And we saw one technique, scanning tunneling microscopy, for seeing atoms. Only when we understand and see atoms, you might think, only then could we, should we, go on to the next level of complexity, to molecules.
>
> Do you think that's true? That development of a field should await complete understanding of its foundations? I hope you don't. We knew the earth was round centuries before an Apollo astronaut took a picture of it from the moon. And we were dead sure of the existence of atoms, and knew just how atoms connected up to form molecules, before those beautiful, clear STM pictures.

> Chemistry, like any human activity, proceeds simultaneously on many levels, with partial understanding, always incomplete, sometimes wrong, incredibly mostly right. A great intellectual achievement of chemistry, of humanity, a chart organizing all the elements, called the Periodic Table, developed fifty years before we knew what the atom is about, is the subject of the next program.

Not only were the directors aghast at what I said, but I also said it well, with feeling. Most of the time I was not good on camera, and there was no money to send me to acting school. So I had their attention, finally. They edited out part of the offensive moon landing-STM sequence; I modified my ending. And we all understood (I think) the point that you don't have to <u>see</u> something to know, for sure, what is in this world

But it was worth it! I am proud that we created the first video course in chemistry ever made. The credit for the programs foes to Izzy Adler, Nava Ben-Zvi, Richard Thomas and all the folks at the Educational Film Center, Gil Castellan, Margot Schumm, Mary Beth Key, Don Showalter, and Ivan Legg. I wish they could have shared in this award.

5

It is time here to reassert my confidence in what we do. We teach chemistry — the art, craft, science, and business of substances (now known to be molecular) and their transformations. We introduce young people to the molecular science, awakening in their minds the ability to deal with the balance of simplicity and complexity that characterizes chemistry. We believe that chemistry instruction at every level must be done in the context of a liberal arts education, fighting compartmentalization all the way and connecting chemistry to economics, literature, history, society, to <u>culture</u>, and to be recognized as culture, in the broadest sense. We believe that the student is best served by consistently being led to value discovery and true understanding. It's not easy, but there is nothing I love more than teaching. As you do. Thanks for honoring me with the Pimentel Award!

Acknowledgment: Significant parts of this lecture are taken from articles I have written, and which have been published in American Scientist, Chemical and Engineering News, Chemistry, A European Journal, Chemistry Imagined (Smithsonian Institution Press), and the Journal of College Science Teaching. I am grateful to Norman Goldberg and Greg Landrum for their help in the construction of this paper.

J. Coll. Sci. Teach

SOME HERETICAL THOUGHTS ON WHAT OUR STUDENTS ARE TELLING US

Feb. 15, 1996

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Abstract: From the ritual of reading students' comments on an introductory chemistry course come some reflections on teaching and learning. Even when we feel that we finally got the course right, in teaching the spirit of the science and the process of its construction, a good number of students tell us what we don't want to hear: that they got along fine by memorizing formulas, and that they don't want all those digressions about science in the real world and in culture. Since we must learn from the students, we examine the validity of their propositions, as much as they run counter to what we want to believe. So we try to analyze why it is that you don't need to understand everything in science (chemistry in particular) to (a) use the science effectively, (b) work as a normal, responsible human being in the world, (c) even to do creative work. And why compartmentalization is an effective learning strategy. We disagree, deeply, but young people are trying to tell us something...

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There is a time, twice a year, when those of us who teach introductory courses sit down in a comfortable chair, pour ourselves a middling portion of single malt Scotch whiskey, and begin to read the comments that students write about our teaching. For the overall ratings, numerical in nature, we can bear to wait – the computer will dutifully compile these single point undifferentiating indicators. What we settle down to read are the "free-style comments", where the students are encouraged to write (anonymously of course) what they think of the book, the exams, and of course, of the lecturer. Many, not all, universities give students the opportunity to express themselves in this way. Some of us have learned to avoid asking silly questions with predictable responses, such as "what is the best part of the course?".

So we sit down, perhaps turning on some Chopin to complement the whiskey, and face those student responses. Many are positive, as (with a trace of mild astonishment) "I didn't think I'd like chemistry, but Prof. Coppola made it fun!", "I actually enjoyed going to the lectures," or "I didn't get a very good grade, but I sure learned a lot." It's not always easy for a student (or us) to say a word of praise, to give thanks graciously harder still.

Positive feelings generally wash over us leaving small marks. Happiness is often diffuse. But pain is sharp – the small pain of a torn cuticle, the stronger incapacitating pain of a broken bone. Or the mental anguish of reading an evaluation such as "Prof. Hoffmann spends all his time on digressions, relating chemistry to politics, history, God knows what else. Who cares how hemoglobin or catalytic converters work? I want to know what's on the MCATS." Or "I got an A by memorizing equations and doing exam problems that were exactly like the problems that I had seen on the previous tests..." Or, "As far as I am concerned I did not need to go to class."

Now this hurts – ergo the whiskey and music; it hurt last time too... Our reaction comes in part from this inability to weigh appropriately emotional praise and criticism. Differentiating among the negative comments, we can easily forgive the simple nastiness of resentment released under cover of anonymity. We are more wounded when the students condemn exactly what we are most proud of in the educational process: we finally got this course right! More than merely the course contents, that neutral list comprising the syllabus, we more importantly developed the spirit of our science (chemistry <u>in</u> culture, and chemistry <u>as</u> culture, as it should be at a liberal arts university) and the process of its construction (stressing understanding and discovery). We finally understood (and thought we succeeded in communicating) that multiculturalism embraces all part of the university experience, and is as inclusive of intellectual constructs, such as chemistry, as it is of the traditional social ones. Then to get such comments really, really hurts.

We could counter, and lash out at the immature young people, at societal pressures and at all the things that make for their wrong attitude toward learning. Better we release our anger on them than on those dear to us... Or we could take another sip of the Lagavulin and reflect on what we can learn from the students' comments, from just those comments that wound most.

As teachers, we invest a great deal of our professional intellectual lives trying to see beneath the surface of what we encounter. What drives our curiosity is trying to understand core phenomena or motivations that give rise to what we see. That is, we try, even if we don't always succeed, to be attentive and insightful learners. For we believe that a high road to effective teaching is to be a good learner when analyzing a students' work or perspective.[1] This is as satisfying an intellectual challenge as authorship or laboratory research.

An effective analogy that one of us (BPC) has created for demonstrating that anybody who takes on the "teaching" role must think (to learn) before despairing about ignorance, is given here:

> *You are teaching multiplication. To probe the students' mastery of the subject, you give an examination. To which one student provides the following answers:*
>
> *2 x 2 = 4*
> *1.1 x 11 = 12.1*
> *3.5 x 1.4 = 4.9*
> *-1 x 0.5 = -0.5*
> *-3 x 0.75 = -2.25*
> *2 x 4 = 6*
>
> *What do you do? You can shake your head and say "How can a student who can multiply noninteger and even negative numbers make such a stupid mistake!" Or you can think about what the student's response is telling you. And revise your educational strategy accordingly.*
>
> *The student has done nothing wrong, except...to think that multiplication is addition.*

Teachers and students meet in the classroom to fulfill the terms of a tacit covenant of instruction. There is more to it than being paid to teach – we sacrifice what else we could be doing during that hour when we teach, or even when we read their comments, to confront a simple question: “Am I being understood?” We learn from books and other media (oh, how imperfectly via these comment sheets!) at our convenience, but in classrooms teachers and the taught come together for just the kind of feedback that is unique to our conversational profession. All classroom pedagogy revolves around ways for the faculty to learn “Am I being understood?” Students want to know this too: “Are we being understood?”

So...we force ourselves to listen to students who have confronted the subject matter and ideas we have so painstakingly (and, we hope, eloquently) provided. But the students have not constructed the same understanding that we have... of the subject, its ambience, and its process. This may be sad, but it is true, as those comments of theirs so painfully reveal. We listen unwillingly, for we are sure that we are right. But we try, because they are right, also. In collaborative communities, the distinction between who is the “teacher” and who is the “learner” becomes blurred, if not wholly imaginary to begin with. Here's what we think we hear:

1. <u>The students are telling us that you don't have to</u>

understand everything in chemistry to make progress in and use the science.

Yes, we'd like them to understand, and we have designed our course so as to emphasize the process of understanding. But learning in chemistry is (a) a curious mixture of proof (real proof), and of belief (accepting on faith, trusting that someone else has proved, or that proof might be forthcoming if one advances in the subject). And that learning is (b) sequential, in an intriguing, intellectually inconsistent way – it proceeds by first understanding something, then memorizing something else, then using the mathematical expression of what was understood in a rote or algorithmic (yes, unthinking) way so as to solve a real problem. We develop a tacit tolerance for the fundamental inconsistencies that define the edges of our understanding. All this, mixed up with occasional necessary bouts of memorization and a nomenclature that has pretensions of being systematic...

As mature learners, we include as many strategies as we can in our arsenal for inquiry. Progress does not occur because we have excluded memorization, but rather because we recognize when memorization is precisely the most effective strategy to use. As much as we would like to enact a truly Socratic dialogue with undergraduates, the reality of teaching thousands of students has made this impossible. It may be that the only potentially authentic thinking in on-your-feet creative situations we place students into are our examinations. Regardless of any rhetoric we provide in class, our examinations transmit the learning objectives that are targeted for comment by students.

Let's take an example: We derive the ideal gas equation, PV=nRT, by historical or experimental appeal to the individual Gas Laws (of Boyle, Charles, and Gay-Lussac). We and the students "understand" the formula (how limited that understanding is, how unreal the ideal, becomes clear in a physical chemistry course). We see the formula in our minds, its beauty in the chemistry and physics it so succinctly summarizes for us. We go on to use it — in a myriad problems, from balloons to equilibria, from determining molecular weights to thermodynamic cycles. And in using it we do <u>not</u> go back in each instance to the derivation. We use it as we need it, as a formula.

The reason we shouldn't get angry at students who says they got by "just memorizing the formula" is that they are just shading their response — very probably they understood a lot, but then chose to emphasize the formulaic use. We think that as much as we value <u>sophia</u> and understanding, that knowledge and learning also involve a component of suspending understanding, or at least pushing it into the background. We ask the reader to recall the problems of twenty-five years ago with "the new math" in primary education.

2. There's an even broader lesson, we think — <u>you don't have to understand everything in order to (a) operate as a normal successful human being in this world, or (b) even to do creative</u>

work of the highest degree.

Once again, we have to begin by saying ever so clearly that we value real understanding, that knowledge is an absolute good. And the special contribution from formal education, schools and universities is centered, we believe, in their being the place where connections between general educational and professional training objectives are constructed and maintained. Elsewhere in life, other imperatives, often economic, dominate.

However, it is clear that technical training is of great pragmatic value even in the absence of the connections forged at a university. Practice and experience suggest that this is the way of the world: we usually learn to use technology's products quite separately from the underlying context, and we can make successful and productive, humane, contributions without even being aware of any appendant knowledge. Driving an ambulance to an accident site does not require a cognitive awareness of the thermodynamics of combustion; the thermodynamics operates just fine without us. We use calculators to help us do arithmetic, and we choose to need to understand how learning arithmetic allows us to make the necessary judgements about the outcomes of button-pushing, while at the same time we choose not to understand things about batteries, liquid crystal displays, the manufacture of silicon chips and the marketing of calculators. Performing a specific task on an assembly line can be done well when the laborer is completely unaware of the other tasks on the line or even the object being assembled. Sometimes that is the learner's choice, quite democratic and informed, also.

Let's jump to the creative act in our science. The synthesis of a new antitumor agent, the perfection of a new industrial process that avoids the use of a harmful solvent, may both involve a heterogeneous catalyst. The catalyst does something reproducible, taking, say, an olefin, and epoxidizing it specifically on one of the two olefin faces. We may have a vague idea how this works on the molecular level, but should we suspend use of the reaction until we really understand the catalyst mechanism? That would be just as silly as to ask Archie Ammons to tells us the metallurgy of the keys of the ancient typewriter that he uses before he writes a poem.

The pressure to understand everything betrays a simplistic reductionist world view. As one of us has expounded (perhaps tiresomely) elsewhere, reductionist (or vertical) understanding is just one way of knowing the world. The other (call it horizontal) way is to understand the world, quasi-circularly if you insist, in terms of the concepts that have evolved in the field under consideration, concepts as complex and seemingly poorly defined as what one is trying to understand.[2] So a telephone that makes a call to an ambulance is accepted as a communication device, working or not working, able to place a call here but not there. It is paralyzing (if not useless) to start to think of the workings of the telephone in a reductionist manner when it is time to call an ambulance. Understanding at some level is definitely needed to fix the telephone, still more complete understanding to create a better telephone.

Jean-Marc Lévy-Leblond makes the important point[3] that we should not wring our hands in despair when we see the results of "ignorometry", all those surveys which show us how ignorant common people are of science, or of history, or of geography.[4] The very same "scientifically illiterate" people drive automobiles pretty well, use word processors, microwave ovens, and lawn mowers. Ignorant by one measure, they know quite a lot of the real world, learning <u>just enough</u> to function as normal, productive citizens. Lévy-Leblond remarks "Should we not start by admitting and admiring these achievements, instead of denying and lamenting the failures?"[5] As scientists, we're not that superior when we interact with machines or tools of higher complexity.

Craig Nelson asks the provocative question: What is the shape of the earth?[6] Two plumb lines separated by any distance on the surface of our planet are not parallel, yet the flat earth assumption is manifest in architecture. What is the shape of the earth? Round? No. A sphere? Hardly. An ovoid? Only if you blur your eyes and don't watch over time. Nelson's point reminds us that our very <u>best</u> theories are only the latest version of Flat Earth, and only better by decimal places of agreement with what is observed, not by "truth" in an absolute sense.

The intrinsic beauty of a model is tied to its ability to function, to deliver useful information upon which we may act.[7] Good models inspire productive experimentation rather than retire lab coats. One important thing to remember about models is a tenet of General Semantics, attributed to Alfred Korzybski: "The Map is not the Territory"[8], which was inspired, according to popular mythology by René Magritte's "This is not a pipe."[9] However heretical (and in one way incorrect) it seems, chemistry instruction would benefit from an explicit understanding that "H_2O" is not "water".[10]

3. Still another lesson from our students, one we don't want to hear: <u>Compartmentalization is an effective strategy for the workings of the world, and may be for learning</u>.

We tell them of the Haber-Bosch process as an example of Le Chatelier's principle at work, and can't pass up (at least some of us can't) talking about catalysts in general, and relating Fritz Haber's tragic story, and how it took the talented engineer Carl Bosch to convert Haber's discovery into a real process, and, for good measure, telling them of nitrogenase as well. We tell the students about solubility constants and illustrate the subject by discussing commercial water softening and the composition of kidney stones. We feel good as we do this, for we have served the goal of a liberal arts university, and have connected up different parts of chemistry. This seems so essential in an age of specialization.

Some students like this. More yawn, and tell us we confuse them with the digressions: "Just tell us what we need to know on the next test..."

They're wrong, of course. The unity of the world, not only chemistry, will catch up with them. The world only looks disintegrated because they learned, from us, that this met their educational needs. After all, we are the ones who chose to write test questions (or textbook chapters) about solubility constants without much mention of their wondrous applications. Our students are only eighteen, too focused in on a profession, and see us as a barrier between them and medical school, or as a useless burden on the way to being an engineer or running a farm.

But in a way they are right. First of all, the lesson of the animal cell or the Volvo assembly line is that specialization and compartmentalization <u>work</u>. There is a reason (efficiency, not divine design) for the nucleus storing the DNA, the potassium channel letting through just that ion and no other. Second, analysis works as a learning strategy, breaking a complex whole — a synthesis of vitamin B_{12} by the body or by Woodward, Eschenmoser and 99 friends, the Haber-Bosch process mechanism — into more comprehensible building blocks (almost an argument for reductionism!) Analysis is inherently compartmentalizing. Third, it is difficult, indeed sometimes confusing, to deal with the whole. Learning the pieces is a strategy for comprehending the whole. You can't see the forest without the trees, either!

The counterargument is clear. The real test of understanding is to use the pieces to build a whole, even more so to construct wholes different from the one we initially disassembled. If you learn only what is in the compartments, or one task on the assembly line, if you don't push your way through to assembly and integration, you...will be stuck in the pieces, on the assembly line.

Schools and universities need to be inclusive of the broadest menu of choices. Craft, knowledge, and cunning have been fragmented – too much so, we think. Universities must be the places where the answers to reintegration's questions can be found. Indeed, even assembly lines have gone reintegrative: in many manufacturing plants workers learn to perform many tasks and, in some cases, groups take collective responsibility for the whole product. Can we do less? Disciplinary separation that leads to cultural isolation threatens to remove reintegrative choices from the menu of formal education. We can choose to do this, _mea culpa_ ... _nostera culpa_; but let us first make sure that we realize there is a decision to be made.[11]

.....

It is time here to reassert our confidence in what we do. We teach chemistry – the art, craft, science, and business of substances (now known to be molecular) and their transformations. We introduce young people to the molecular science, awakening in their minds the ability to deal with the balance of simplicity and complexity that characterizes chemistry. Both of us believe that chemistry instruction at every level must be done in the context of a liberal arts education, fighting compartmentalization all the way and connecting chemistry to economics, literature, history, society, to culture, and to be recognized as culture, in the broadest sense. We believe that the student is best served by consistently being led to value discovery and true understanding, rather than being restricted to memorization as the only way of knowing. And, yes, we take a paternalistic viewpoint that we – not the two of us, but the community – know a little more than the student of what is essential and valuable in the science taught.

It has grown dark. A second glass of that marvelous Scotch brew of water and grain (a little bit of chemistry, too), tasting of peat and iodine, the color of heather on the hills at a certain time of year, that second glass will get us in trouble. It's time to finish reading what our students say. And perhaps we don't need that second glass, for even as we know that we have taught well, taught what needed to be taught – even if we did all we could and did it well, we still can learn something from our students.

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A Chemist Helping Chemists

April 30, 1996

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Ithaca, NY 14853-1301

Dear Roald:

As you will see from the enclosed menu of my talks, I have included one on Chemophobia. That talk incorporates most of my Parsons Award address, which was published recently in *The Chemical Intelligencer*, copy enclosed. It also incorporates some wonderful passages from you, and I wonder exactly how you would like those passages cited.

With many thanks for your help and best personal regards, as always,

AB/cw

Enclosures

Dr. Alfred Bader
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A Chemist Helping Chemists

April 3, 1996

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

Thank you so much for your delightful letter of March 27th and the essay dealing with camels and the Pentagon. I hope it will not be the last chapter, but these are so good that I fear I will always say that, and of course, somewhere you will have to stop.

The only comment I have relates to your page 7, referring to Doray's depiction of Joseph sold by his brothers. As you will see from a 1976 publication written by me, I don't believe that the brothers really sold Joseph, although they certainly planned to do that initially.

I also love the painting, which I am convinced depicts Professor Brande teaching Faraday to make Prussian blue. It is probably the finest painting of historical chemical interest that I have ever owned.

It belonged to a dealer of armaments - guns, etc. - in the South, and he hoped to get $100,000 for it, based on his belief that the teacher is Davy and the painting is by Thomas Sully. He had some relevant correspondence from the Met, which I am convinced is mistaken. He did not know that the experiment was making Prussian blue, but I did that very same experiment myself and have no doubt.

It took me over two years to convince him to be somewhat more reasonable in price, but then when he brought me the painting to Milwaukee, he refused to accept my check. I told him that that was no problem, as we could go to my bank and have it certified. His reply was that he didn't worry about my check; he worried about the IRS knowing of his getting such a large check. Well, after taking counsel with Marvin Klitsner and checking that he had good title to the painting, I did pay him in cash and of course, got his receipt.

Since then, I have learned a great deal, particularly about Faraday's intense interest in Prussian blue and his long friendship with Brande.

I hope that you will have a really good Passover.

With fond regards from house to house, as always,

AB/cw

Enclosures

Cornell University

Department of Chemistry
Baker Laboratory
Ithaca, New York 14853-1301 USA

March 27, 1996

Dear Alfred,

I'm so happy that you liked those two chapters, for I worked very hard on them. Someday I'll tell you how they are written, or who wrote what.

Shira and I appreciate the corrections. There is now plenty of time, because we missed a deadline to publish this year, and so it will be in mid-1997, for my 60th birthday. The versions you saw were drafts, and in the final version there will of course be all the references.

You can then haggle with Freeman (the publisher) for a discount.

Soloveichik did not write much, but he was very acute, and broadly educated. I've come to admire him immensely, and I'm only sad that I was not interested in these things when I could have spoken with him...

On the Bar Ilan responsa collection; it's only a [illegible]oke in part. I have used the computerized file, and it is *very* useful. But not that easy to search it.

I've ordered the Langston + Palfreman book.

Of course please feel free to quote anything you wish from our drafts. The last chapter has just reached first draft stage (attached). And who knows maybe it won't be the last in the book, but will be pushed ahead. I do not ~~to~~ intend to write more chapters ~~about~~, but it could be this one would be better earlier. So you are really seeing a work in progress!

I'll ask Shira about the use of human embryo tissue for Parkinsons.

I love the painting, and you must be right, it's Faraday. How did you locate it?

Be well, friends.
Roald

Dr. Alfred Bader
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A Chemist Helping Chemists

March 19, 1996

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

I had to smile when I read your card saying "I don't mean to impose a burden of reading ... ".

I so enjoy reading your essays, and now I believe that I have read all of them except the one dealing with camels and the Pentagon.

When the book is out, I will inquire whether I could perchance get a special price if I purchase 10 or 20. They will make wonderful gifts.

What few comments I have would all have been classified when I was a boy in Vienna as *Wichtigmacherei*. These points are so simple that I have simply Xeroxed the pages with the few notes.

The end of the play, "Where is Yigal?", is absolutely brilliant.

Have you heard the joke making the rounds in Israel: Bar Ilan University now has a computer printout capability to all references and opinions in the Talmud. Thus, if you have a question, you can get the answers. There is yet another program that if you have a question will give you the names of rabbis who will give you the answer you want.

Have you read the book, "The Case of the Frozen Addicts" by Langston and Palfreman, ISBN 0-679-42465-2? That book would not have been written if I hadn't purchased a kilo of MPTP in a suburb of Montreal many years ago.

I am very curious to know what Shira thinks of using human embryo tissue to treat people with Parkinson's disease. Rabbi Jay David Bleich of the Cardozo Law School is against it, but I am not at all certain that he is right.

I have been asked to give talks on Chemophobia, expanding the talk I gave at the ACS meeting in Anaheim last April when I received the Parsons Award. I hope that you will not mind if I incorporate your and Rabbi Soloveitchik's thinking about the two atoms and your discussion about CFC's in my talk, of course, citing your work.

I was most interested in your discussion of the rabbi of Radzin making Prussian blue. Did you know that Michael Faraday was exceedingly interested in this? I am just working on a painting which I believe depicts Brande teaching Faraday to make this dye and the relevant correspondence might interest you.

Please, Roald, don't let anybody persuade you to remove the art from your essays.

When will we see you in Milwaukee? I have so many new paintings to show you.

With fond regards from house to house, as always,

AB/cw

Enclosures

Roald Hoffmann and Shira Leibowitz

Pure/Impure

New England Review
1994, 16(1): 41–64.

File

I have made you an assayer of my people
—A refiner—
You are to note and assay their ways.
They are bronze and iron
They are all stubbornly defiant;
They deal basely
All of them act corruptly.
The bellows puff;
The lead is consumed by fire.
Yet the smelter smelts to no purpose—
The dross is not separated out.
They are called "rejected silver,"
For the Lord has rejected them.[1]

The Book of Jeremiah 6:28–29

LEIBOWITZ: In this jeremiad, the prophet berates his people for having gone astray. His language is strong, high, and poetic. And it is interspersed with several passages which indicate substantial familiarity with metallurgy.

An interpretation has been provided by the much-maligned former American President, Herbert C. Hoover, who was a talented, unusually well-educated mining engineer, and by his wife, Lou H. Hoover.[2, 3a,b] The Hoovers discern in the Jeremiah passages the ancient process of cupellation: an impure mixture of silver or gold with undesired admixtures is melted in a cupel, a shallow dish shaped from bone ash. Lead is added. A blast of air oxidizes the non-precious metals. The base metal oxides dissolve in the lead oxide, which is skimmed off, leaving behind the pure silver or gold. Jeremiah invokes the process metaphorically; the wickedness of his people is so great, they will not be purified. The Hoovers remark:

> From the number of his metaphors in metallurgical terms we may well conclude that Jeremiah was of considerable metallurgical experience, which may account for his critical tenor of mind.[4]

Jeremiah's stern criticism caught our eye in its conjoining of a scientific or technological argument and an appeal to purity, a condemnation of mixture. Purity is a traditional feature, indeed a desired goal, of religious systems.

HOFFMANN: That passage from Jeremiah is not as clear as you think. If toward the end the prophet uses a powerful metallurgical metaphor for purity, he undermines

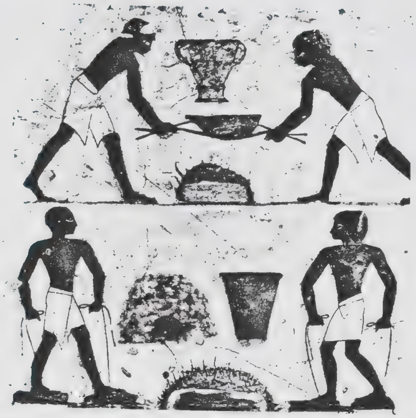


Illustration 1. Wall mural from the grave of Rekhmire at Thebes. 15th Century BCE, showing refining (of gold?) and the foot-driven bellows for smelting. Jeremiah was familiar with these processes.

his aim by invoking iron and bronze near the beginning. Jeremiah's assessment of these metals as "stubbornly defiant" (emphatically repetitive in Hebrew, *sorerey sorerim*) admits their strength, as materials.[5]

And why are they strong? *Because* they are impure, mixtures, alloys. I suspect that Jeremiah, good metallurgist that he was, knew that bronze, in the swords and ploughshares of the Israelites, was a mixture of copper and another metal, tin. And carbon in iron strengthens it; properly processed it becomes steel.

Science teaches us that nothing is pure; moreover that complete admixture is the natural course of events. And chemistry gives us abundant examples of superior impure materials.

So religion squares off against science once again, purity vs. impurity. Or so it seems . . .

I. RELIGION AND THE ASPIRATION TO PURITY

COLETTE: As that word "pure" fell from her lips, I heard the trembling of the plaintive "u," the icy limpidity of the "r," and the sound aroused nothing in me but the need to hear again its unique resonance, its echo of a drop that trickles out, breaks off, and falls somewhere with

> a plash. The word "pure" has never revealed an intelligible meaning to me. I can only use the word to quench an optical thirst for purity in the transparencies that evoke it—in bubbles, in a volume of water, and in the imaginary latitudes entrenched, beyond reach, at the very center of a dense crystal.
>
> *The Pure and the Impure*[6]

HOFFMANN: Words such as "pure" and "impure" carry a multitude of meanings. The sense least encumbered with moral connotation is that describing the distinction between objects composed of one substance versus those consisting of a mixture of several. So Vicks Throat Lozenges are a mixture of benzocaine, cetylpyridinium chloride, menthol, camphor, eucalyptus oil, D&C Red No. 27, D&C Red No. 30, flavor, polyethylene glycol, sodium citrate, sucrose, and talc. D&C Red No. 27 is tetrabromotetrachlorofluorescein; D&C Red No. 30 is 6-chloro-2-(6-chloro-4-methyl-3-oxo-benzo[b]thien-2(3H)-ylidene)-4-methyl-benzo[b]thiophen-3(2H)-one, alias "helindone pink CN."[7] "Flavor" certainly contains several molecular components. Other examples of mixtures are your breakfast cereal (read the ingredients!) and pure mountain spring water (*certain* to contain, at the parts per million level, calcium, magnesium, chloride, sodium, sulfate, bicarbonate, and organic matter, and at the parts per billion level all kinds of things you don't want to know about, such as ammonia, borate, fluoride, iron, nitrate, potassium, strontium, aluminum, arsenic, barium, bromide, copper, lead, lithium, manganese, phosphate, and zinc).[8]

From that reasonably neutral starting point of mixture, the meaning of "pure" and "impure" develops. First, there is a metaphorical movement to the realm of the emotions, carrying with it a certain confusion with the ideas of concentration and intensity. A saint, Buddhist or Christian, who meditates intently, is pure in soul. He is not distracted; she is intense.[9]

Second, the movement to the figurative sphere inevitably triggers the association of a positive ethical or moral value to the pure, and a negative one to the impure. To be spotless, unblemished, to be pure in mind, is to approach godliness. "How blest are those whose hearts are pure: for they shall see God," it says in the Sermon on the Mount,[10] echoing the 24th Psalm:

> Who may ascend the mountain of the Lord? Who may stand in his holy place? —He who has clean hands and a pure heart, who has not taken a false oath by My life or sworn deceitfully.

To be pure is to testify to the holiness of God and his people. Purity becomes symbolic, good and *of* God.

LEIBOWITZ: Is there any doubt that purity is a positive good of religion? It is an important factor behind the complex rituals and regulations governing marriage, inheritance, sacrifice, and cooking. Entire tractates of the Talmud, that rich body of initially oral law governing the behavior of observant Jews over 2000 years, are devoted to the rules and regulations of ritual and physical purity. To an outsider the discussion might seem esoteric, a debate between rival rabbinical schools as to how many drops of milk accidentally spilled into a veal stew will cause the dish to become thereby a forbidden milk/meat mixture. But for the Jewish people, every act must be a sancti-

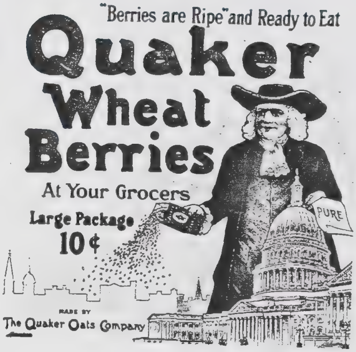


Illustration 2. A 1910 advertisement for Quaker Wheat Berries touting their purity. (Warshaw Collection of Business Americana. Archives Center. National Museum of American History. Smithsonian Institution.)

fication of His holiness. The exhortation to purity is there in the Torah, the Five Books of Moses:

> You shall be holy, for I, the Lord thy God, am holy . . . You shall observe My laws. You shall not let your cattle mate with a different kind; you shall not sow your fields with two kinds of seed; you shall not put on cloth from a mixture of two kinds of materials [*shaatnez*].
>
> Leviticus 19:2 and 19

Rationalist attempts to find hygienic or scientific arguments for these rules, or to seek their economic origin abound. So in *shaatnez,* the prohibition of mixing wool and linen, some people see the ancient struggle between shepherds and farmers. But while these explanations are ingenious, tracing the inevitable interrelatedness of the spiritual and physical world, the reasons for the ubiquity of proscriptive ritual must be deeper.

Illustration 3. The search for *shaatnez,* the forbidden mixture of wool and linen, often uses the tools of modern science. Here is a view of a Brooklyn *shaatnez* laboratory. (Photo courtesy of Cary Sol Wolinsky.)

> MARY DOUGLAS: Defilement is never an isolated event. It cannot occur except in view of a systematic ordering of ideas . . . The only way pollution ideas make sense is in reference to a total structure of thought whose key-stone, boundaries, margins and internal lines are held in relation by ritual of separation . . . To be holy is to be whole, to be one; unity, integrity, perfection of the individual and of the kind. The dietary rules [in Leviticus] merely develop the metaphor of holiness on the same lines . . . the underlying principle of cleanness in animals is that they shall conform fully to their class. Those species are unclean which are imperfect members of their class, or whose class itself confounds the general scheme of the world.
>
> *Purity and Danger,* Ch. 3, "The Abominations of Leviticus"[11a]

HOFFMANN: In her perceptive 1963 book *Purity and Danger,* Mary Douglas views rites avoiding pollution or impurity as ritual demarcations of the normal from the unnatural. Douglas notes that what disturbs the Lele people of the Congo region about the scaly anteater is that it is *as an animal* abnormal—it is egg-laying, but suckles its young; it is scaly like a fish, but climbs trees; its young are born singly, as those of humans. She constructs a plausible parallel argument for a cultural basis of the prohibited animal species of the Jews, the so-called abominations of Leviticus.

Douglas goes on to argue persuasively that "where the social system requires people to hold dangerously ambiguous roles, these persons are credited with uncontrolled, unconscious, dangerous, disapproved powers—such as witchcraft and evil eye."[11b] The disordered, or that simply outside the ordered, is not just static and expelled. It spells danger to a stable society. Danger is power.

For a stable society, or a stable form of matter, danger may be as simple as change. In a phase transformation, the precipitous change of one form of matter to another (for instance water to steam or ice), the beginning (nucleation, as it is called) is always at a locus of disorder, or an impurity.

LEIBOWITZ: Douglas correctly describes the immense importance of separation in the Biblical scheme, and its relationship to purity and holiness. This idea is articulated in the blessing said at the end of the Jewish Sabbath, setting it off from the weekdays:[12]

> You have graced us with intelligence . . . You have distinguished between the sacred and the secular, between light and darkness, between Israel and the peoples, between the seventh day and the six days of labor . . . Our Father, Our King, begin for us the days approaching us . . . free from all sin, cleansed from all iniquity.

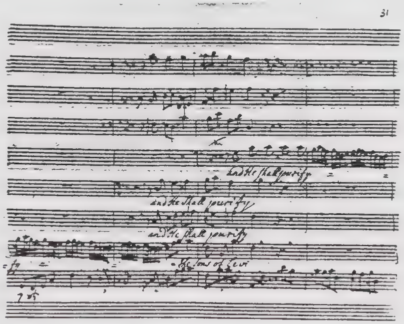
But an anthropologist analyzing the terminology of purity in a foreign culture through the veil of English will be handicapped.

First of all, highly developed religious systems do make a definite distinction between physical and ritual impurity.[13] Thus in Hebrew we have *tahor*—pure, clean physically (and spiritually, by metaphoric extension). This can be negated, as *lo tahor*—impure, not clean physically and spiritually. But spiritual defilement, pollution, is described by another adjective, *tamey*. The Biblical candelabra were made of pure (*tahor*) gold, but these might or might not be *tamey*, depending on their contact with a source of defilement (a corpse, a reptile, etc.).[14]

Even if an anthropologist studies a culture in terms of its own language, she may be comparing—really confusing—concepts which seem similar but aren't. There are Biblical laws which superficially seem to be about the same concerns: mixtures and impurities. These laws are gastronomic (meat/milk, leaven/non-leaven); about fabric (linen/wool); animal breeding (horse/donkey); marriage (Israelites/neighboring pagan peoples); temporal (*eruv tavshilin,* mixing of holidays and Sabbaths); geographic (*eruv tehumim,* mixing of public and private domains); and metaphysical (impurity due to proximity to sources of ritual defilement). But each concept is embedded in its own legal infrastructure from which it cannot be extricated and compared with others out of their contexts.[15]

This problem is endemic to anthropological approaches. In a deconstruction of Indian marriage laws, Wendy Doniger recently observed that "the attempt to rationalize other people's apparent irrationalities is a game that many scholars of religion have enjoyed playing, particularly . . . in this era of moral relativism."[16]

Ultimately, the strong claims of religions do not depend on what men and women call reason. This has been the conclusion of Jewish thought—witness the Book of Job, or Rav, a 3rd-century sage, who commenting on a passage from Psalms (18:31), "the Lord's utterance is pure," asserts, "What difference does it make to the Holy One whether one eats unclean or clean substances? It follows that the commandments were given only to purify people."[17]

GEORGE FRIDERIC HANDEL:[18]

HOFFMANN: The connection between purity and religious aspiration is awesome. Listen to George Frideric Handel in an oratorio where he set several lines of the prophet Malachi's call to the music of thirty singers and an equal number of instruments:

And who shall stand when he appeareth?
For he is like a refiner's fire,
And like fuller's soap;
And he shall sit as a refiner and purifier of silver;
And he shall purify the sons of Levi,
And purge them as gold and silver.

Malachi 3:2–3

Jeremiah was not the only prophet who knew metallurgy.

II. SCIENCE AND THE DRIVE TOWARD IMPURITY

NICOLÁS GUILLÉN:

I am not going to tell you that I am a pure man.
Among other things
we have yet to know if what is pure exists.
Or if it is, say, necessary.
Or possible.
Or if it tastes good.
Have you ever had chemically pure water,
laboratory water,

without a grain of dirt or excrement,
without a bird's small excrement,
water composed only of oxygen and hydrogen?
Puah! What filth!

I do not say, then, that I am a pure man,
I will not tell you that: everything to the contrary.
That I love (women, naturally,
for my love can speak its name),
and like to eat pork with potatoes,
and chickpeas and sausages, and
eggs, chicken, lamb, turkey,
fish and clams;
and I drink rum and beer and brandy and wine,
and fornicate (even on a full stomach).
I am impure, what can I say?
Absolutely impure . . .

From "I Declare Myself an Impure Man"[19]

HOFFMANN: When a chemist runs any reaction in the laboratory or when he or she sees some immunosuppressant activity in an extract from a fungus, the product at hand is almost certainly a mixture. Guillén's "water composed of only oxygen and hydrogen" indeed not only tastes flat to us but is unnatural.

Why all that impurity? In the realm of the living, that's an easy question to answer. A living organism is complex. Even within one specialized cell there are thousands of chemical reactions going on. The multitude of tasks accomplished is staggering—can I begin to describe what transpires as the energy of light and water and carbon dioxide combine in a chain of reactions in which we have identified dozens of steps (and a role for iron, copper, manganese, and magnesium) on the way to a sugar molecule in a lily-of-the-valley?[20a] More than the 100 or so elements, it's the millions of molecules that we sculpt from them that shape the chemistry of the universe. The complexity of plants, our own complexity, demands variety. Two hundred seventy-five constituents have been identified in rose oil, a certain rose essence extract.[20b]

So mixtures and impurity are natural. More than that—there is a natural drive to *maximize* mixing, called entropy.[21] It's not a matter of seeking actively for the most messy state of the universe. It's simply the democratic principle of all possible states being equally likely. Even with small numbers the tendency to disorder is evident. If you toss a coin three times you will get one of the equally likely results HHH, HHT, HTH, THH, TTH, THT, HTT, TTT. (H = heads, T = tails). The two "pure" results (HHH, TTT) are unlikely, *not* because on a given toss there is a preference for a single head or a single tail (they're equally likely for the fair coin assumed). The net outcome of three heads or that of three tails is rare (≡ unlikely, improbable) because each represents only one of eight possible equally likely outcomes. Imagine for 10^{23} coins (that's how many molecules there are in a slurp of water) how improbable it is that all 10^{23} should give heads on a toss! As improbable as that a toss of a properly mixed Caesar salad should lead to three kinds of lettuce neatly segregated, the anchovies on top, the cheese underneath, the egg reconstituted, croutons all together.[22]

It's not far from an identification of the pure with the good to the impoverishing notion that behind every observable of this world is a single cause. In biology, as Thomas Eisner has mentioned to us,[23] such ideas have positively inhibited understanding. Take the one gene-one enzyme theory, or the assumption that each pheromone must be a single molecule.

Insects have a chemically rich communication system. Sometimes a male of a species can detect a handful of molecules of one kind wafted by a female among billions of extraneous molecules. Such pheromones have been sought and isolated, a triumph of modern chemistry.

The story of the sex pheromone of the cabbage looper moth, *Trichoplusia ni*, is instructive. The pheromone was first (1966) thought to be a single molecule ((Z)-7-dodecenyl acetate). Then in 1980 a second crucial component was identified, and in

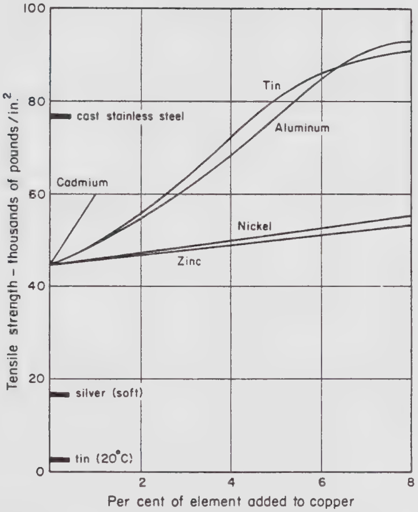


Illustration 4. The influence of metal impurities (alloying) on the tensile strength of cold-rolled copper. (After *Copper Data* 1936, British Copper Development Assoc., London.) The bars at left indicate the tensile strength of tin, silver, and one kind of steel. Note that bronze (copper alloyed with tin) is stronger than either pure copper or pure tin, and may be as strong as steel.

1984 a clue in the way the main component was synthesized by the insect caused Bjostad, Linn, Du, and Roelofs to seek other components, finally demonstrating that a total of no less than six molecules was involved.[24] The western pine bark beetle, an economic pest, has an aggregation pheromone, a mixture that signals all comers, male or female, of that species, to assemble. It is a blend of three molecules: one from the male, one from the female, and one, remarkably enough, from the tree.[25] These are not isolated examples; most pheromones are blends.

The entropy of the universe increases. We may be able to reverse that trend locally, grow a nearly perfect crystal, to write a poem, bring a child to term. But this can be done only with an input of energy, at a cost. A price that makes some other part of the universe messier.

ROBERT LOUIS STEVENSON (from Henry Jekyll's full statement): My provision of the salt, which had never been renewed since the date of the first experiment, began to run low. I sent out for a fresh supply, and mixed the draught; the ebullition followed, and the first change of colour, not the second; I drank it, and it was without efficiency. You will learn from Poole how I have had London ransacked; it was in vain; and I am now persuaded that my first supply was impure, and that it was that unknown impurity which lent efficacy to the draught.

The Strange Case of Dr. Jekyll and Mr. Hyde[26]

HOFFMANN: Not only is there a natural tendency to mix, but chemists and physicists are constantly made aware of the occasionally superior properties of imperfect, disordered matter (glass is such), or of composites. This was certainly appreciated by the metallurgist side of Jeremiah, familiar with bronze and brass, knowing solders and precious metal alloys. Bronze, an alloy of copper and tin (or other elements; the first bronzes were alloys with arsenic), has mechanical properties superior to either pure metal. It was common in the weapons, tools and decorative objects of the Biblical period. Pure metals, and even more so alloys, are strong and ductile precisely because of the existence of imperfections (called "dislocations") in their structure.[27]

A SUMERIAN DISPUTATION: Silver, only in the palace do you find a station, that's the place to which you are assigned. If there were no palace, you would have no station, gone would be your dwelling place . . . In the [ordinary] home, you are buried away in its darkest spots, its graves, its "places of escape" [from this world]. When irrigation time comes, you don't supply man with the stubble-loosening copper mattock, that's why nobody pays any attention to you! When planting time comes, you don't supply man with the plough-fashioning copper adz; that's why nobody pays any attention to you! When winter comes, you don't supply man with the firewood-cutting copper ax; that's why nobody pays any attention to you! . . . Silver, if there were no palace, you would have neither station nor dwelling place; only the grave, the "place of escape," would be your station.

Copper's speech to Silver[28]

LEIBOWITZ: The above text dates to about 2000 B.C.E. It is a "debate" between silver and copper. It may be that copper here really stands for a copper alloy, arsenical copper or bronze, more likely to have been used in tools than native copper by this time.[29]

This debate is not unique in Sumerian literature. The Sumerians were a combative, verbally aggressive people. We have evidence of this in their texts, their litigiousness

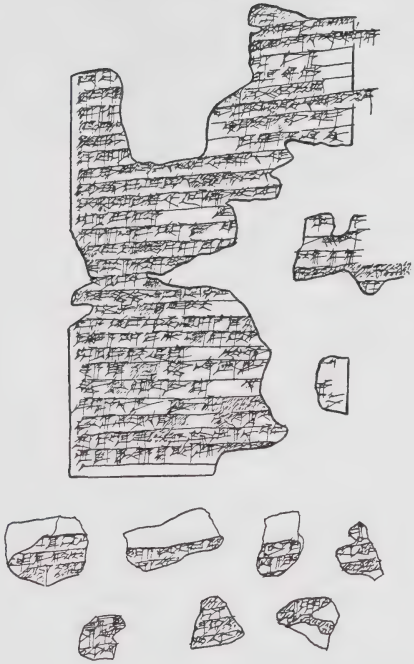


Illustration 5. A transcription of one of the cuneiform tablets of the disputation between copper and silver. The original tablet is in the University Museum, University of Pennsylvania. (Reproduced from the *University Museum Bulletin,* 17, No. 2, Dec. 1952.)

and legal codes. The level of verbal invective and confrontation in their surviving writings is remarkably high.

CYRIL STANLEY SMITH: No metallic material has had more influence upon man's history than iron and its simple alloy with carbon, steel . . . Steel differs in composition from pure iron essentially only by the presence of a small amount of carbon . . . The relation between properties and compositions was fairly clear in the case of the bronzes . . . The fact that steel was also an alloy was not so clear; indeed it was not definitely accepted until the very end of the eighteenth century [of our era!], 3000 years after the practical discovery. This knowledge arose out of and contributed to the Chemical Revolution in an intimate way.

The Discovery of Carbon in Steel[30]

HOFFMANN: An instructive story of the resistance of science to the evidence of the senses (and their extension, instruments) is to be found in the history of the establishment of the correct composition of steel. The material is not new—think of medieval Japanese swords, or Damascus steel. Steel is an alloy, but—and this was a large part of the difficulty metallurgists faced in thinking about its structure—not an alloy of a metal, iron, with another metal. Steel is an alloy, an intimate mixture on the atomic level, with a non-metal, carbon. And the carbon sneaked in, so to speak, through the carbonaceous fuel used in the inevitably intimate contact of heating. Moreover, the optimum admixture of carbon into iron is small, no greater than 1.5%, so it was difficult to detect.

Cyril Stanley Smith, a metallurgist very much interested in the interface of science and art, tells beautifully the story of the establishment of steel as an iron-carbon alloy. In the early part of Smith's story the scientists and philosophers don't come off too well:

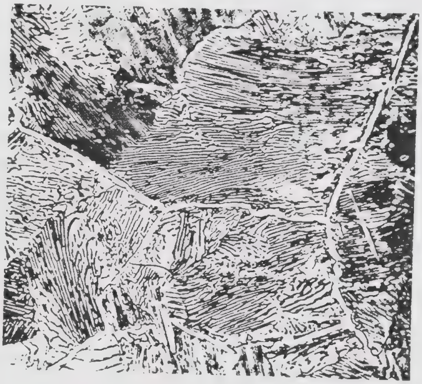


Illustration 6. Photomicrograph of a typical, strong, carbon steel. In this structure there may be seen lamellae (layers) of iron (with some carbon dissolved in it, called ferrite) and iron carbide (a compound Fe_3C, cementite). (Reproduced, with permission from Donald S. Clark and Wilbur R. Varney, *Physical Metallurgy for Engineers*, 2nd ed. [Princeton: D. Van Nostrand, 1962], 123.)

At the end of the seventeenth century, then, we have the practical man (guided as he always will be by the knowledge in his fingers and his eyes) unconsciously putting carbon into iron by his steelmaking processes, while the philosopher thought that some deleterious principle was being removed.[31]

The story unfolds contemporaneously with the ascendance and passing of an erroneous but plausible theory of chemical reactivity, phlogiston. Experimentation and that theory (despite its being wrong) convinced people correctly that something was being added to iron to make steel. Next, practical observation and careful analysis led Swedish chemists to conclude that what was present besides iron was a carbonaceous residue called "plumbago." Interestingly, the earliest written record of carbon in steel is in John Pettus's *Volatiles from the History of Adam and Eve,* which mentions "charcoal" unconsumed by fire rising out of molten cast iron and uses this as a metaphor to bolster man's hope for resurrection.[32] In France, in the years just before the Revolution, within the framework of a revolutionary theory of chemistry, the admixture in steel was identified as carbon.

MIRCEA ELIADE: It has been established that among miners, rites calling for a state of cleanliness, fasting, meditation, prayers, and acts of worship were strictly observed. All these things were ordained by the very nature of the operation to be conducted because the area to be entered is sacred and inviolable; subterranean life and the spirits reigning there are about to be disturbed; contact is to be made with something sacred which has no part in the usual religious sphere—a sacredness more profound and more dangerous. There is the feeling of venturing into a domain which by rights does not belong to man—the subterranean world with its mysteries of mineral gestation which has been slowly taking its course in the bowels of the Earth-Mother.

The Forge and the Crucible[33]

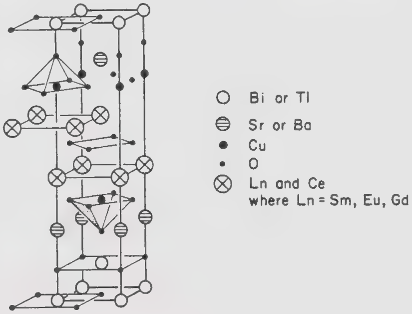
HOFFMANN: Eliade proceeds to cite numerous examples of miners, smelters, and smiths purifying themselves as they prepared to make metals. There is an anthropological and religious dimension to the art of winning metals from their ores and alloying them, as evidenced by the elaborate rituals surrounding primitive mining and metallurgy.

Extending to inanimate ores and metals the life-giving sexuality of the biological world made eminent sense. The idea was especially strong in China, given that civilization's philosophical acceptance of the *yang* and *yin* cosmological principles and its metallurgical skills. The "marriage of metals" that is alloying is an ancient notion, reflected, as Eliade points out, in the *coniunctio* or *Chymical Wedding* of alchemy. And perhaps in another guise in Hegelian dialectic.

Scientists continue to make happy marriages of the elements. In the 1980's a new class of materials was synthesized. It was ceramic in nature and conducted electricity without resistance at temperatures much, much higher than other previously known superconductors. The first superconductors, discovered early in this century, were pure metals. The world record holders until recent times had been alloys of two elements. The new superconductors are compounds of four, five, or even six elements.[34]

Illustration 7. A view of the Chymical Wedding, Conjunction, from the *Viridarium Chymicum* . . . of Daniel Stolcius de Stolcenberg, 1624. (Reproduced from "Chymisches Lustgärtlein," published by Wissenschaftliche Gesellschaft, 1987.)

Here is a structure of one of these superconductors. Not only are there several elements in it, but for the ceramic to exhibit its properties a certain departure of the oxygen concentration from an integral atom ratio, a certain measure of nonstoichiometry, as it is called, is needed. So the superconductor is not only a mixture, but also "imperfect," departing from the simple composition our naive minds want it to have.



Superconductors, superalloys. Conferring power, if not danger. Or maybe danger, too, steel in the unpredictable hands of man. It seems that nature is following Mary Douglas's vision of the impure imparting power.

LEIBOWITZ: Given all this, you might imagine that scientists should come out clearly on the side of mixing, disorder, and impurity; whereas the stance of religion, to which we already alluded, would be the opposite, advocating a pure soul and body. But things are not so simple.

III. THERE IS ALSO ASPIRATION TO PURITY IN SCIENCE

HOFFMANN: The extraordinary properties of some substances emerge only when they are pure. Examples are polymers, such as polyethylene (used in food wrap and a myriad other products), which are stronger when they are crystalline and pure. Silicon, in computer chips and transistors, has to be made exceedingly pure before it exhibits its immensely useful semiconducting properties. But then, to confound things, the pure silicon is "doped" by "impurity atoms" (roughly one impurity to every 10^7 atoms of silicon). This enhances the electronic efficiency of the purified silicon by many orders of magnitude.

Our favorite metal, copper, whose strength was increased by an admixture of tin (or aluminum, or nickel, see Illustration 4), has its prized electrical conductivity decreased by the very same alloying. The purer the copper, the better it serves us, electrically.

> **THOMAS MORTON:** Underlying everything we do is the notion of a pure compound—without that concept we'd be powerless (which is one of the obstacles in studying olfaction, since subjectively "pure" odors are often complex mixtures, while chemically pure compounds often possess subjectively "complex" odors). The definition of purity allows us to function with purpose.[35]

HOFFMANN: What Morton, a thoughtful organic chemist, says has both historical and philosophical import. Chemistry developed by refining methods of separation, isolation, and purification. If we need to worry about harmful dioxins at the parts per billion level, we must have methods of detecting and identifying them in a complex mixture.

Philosophically, it is impossible to define impurity in the sense of mixture, without the notion of purity or the unmixed. Only the establishment of one substance as a pure compound allows one to call another a mixture.

Recall the *blend* of chemicals that characterizes a typical natural insect communication system, the cabbage looper moth sex pheromone, mentioned above.[24] Roelofs and coworkers identified six molecules, in definite proportions, as being necessary. How did they do so? By synthesizing all six separately, then concocting blends that would elicit male flights against an opposing air stream in a wind tunnel.[36]

In science, especially in chemistry, we are continuously engaged in the dialectic of purity and are made aware of the complementary claims of the simple and the mixed.

IV. MIXTURES AND IMPURITY IN RELIGION

> Preliminary morning service: The incense was composed of the following eleven kinds of spices: balm, onycha, galbanum, and frankincense, seventy *minas'* weight of each; myrrh, cassia, spikenard, and saffron, sixteen *minas'* weight of each; twelve *minas* of costus; three *minas* of an aromatic bark; and nine *minas* of cinnamon. [Added to the spices were] nine *kabs* of Karsina lye, three *seahs* and three *kabs* of Cyprus wine—if Cyprus wine could not be obtained, strong white wine might be substituted for it—a fourth of a *kab* of Sodom salt, and a minute quantity of *ma'aleh ashan* [a smoke-producing ingredient]. Rabbi Nathan says: A minute quantity of Jordan amber was also required. If one added honey to the mixture, he rendered the incense unfit for sacred use, and if he left out any of its ingredients, he was subject to the penalty of death.[37]

LEIBOWITZ: While this admonition to good practice upon penalty of capital punishment should be posted in all chemistry laboratories, the recipe given clearly describes the blending of a ritual prescription, of a mixture. The quoted passage from the morning service, originally in the Talmud, is striking counterevidence to the seemingly inevitable emphasis on purity in religious ritual.[38, 39]

Nothing can be omitted, not even the foul-smelling galbanum. Its admixture serves the Talmud as a morality metaphor:

> A prayer quorum in which none of the sinners of Israel participates is no prayer quorum; for behold the odor of galbanum is unpleasant, yet it was included among the species for incense.[37]

Another example of required mixtures: In normal clothing, the observant Jew should avoid the forbidden mixture of wool and linen, *shaatnez* as we mentioned earlier. But in Exodus 28, in the detailed prescriptions for building the Tabernacle and the attendant rites, the robes of Aaron and his sons, the priests, are to be woven with gold; violet, blue, and scarlet wool yarn; and fine linen, all five materials twisted in each thread.

The fact that linen/wool *shaatnez* mixtures are, according to the circumstances, sometimes forbidden and sometimes required, suggests that there isn't anything intrinsically bad—or good—about such combinations. Maimonides puts this philosophically when he places these precepts under the rubric of the command to control one's desires:

> A man should conquer his passions, and is warned not to say, "By nature, I do not lust after prohibited things . . . I am repulsed by meat mixed with milk, I am repulsed by *shaatnez,* I am repulsed by forbidden sexual unions." Say instead, "They are attractive but what can I do? My Father in Heaven has forbidden them!"[40]

In its penchant for specificity, the Talmud deals repeatedly with the problem of defining loss of purity by mixture with the impure. Depending on the sanctity of the commandment, either a majority rule applied, or the prohibited object had to be nullified by a large excess, 60 to 1, of the allowed or pure. In some cases, as for leavening in Passover, no nullification was possible.[41] There is an interesting analogy here to the Delaney Clause, a controversial amendment of the US Federal Food, Drug and Cosmetic Act, which in principle banned the addition to food of all substances that were shown to be carcinogenic, at *any* level, in humans or test animals.[42]

Coca-Cola Now Kosher For Passover

Coca-Cola

קאקא קאלא כשר פיר פסח

Rabbi TOBIAS GEFFEN

Illustration 8. The certification (in English and Yiddish) that Coca-Cola® is kosher for Passover. (From "Lev Tuviah," edited by Joel Ziff, published by the Rabbi Tobias Geffen Memorial Fund in 1988.)

HOFFMANN: In evaluating the permissibility of admixture, rabbinical law made a substantive distinction between intended and fortuitous acts. There's a wonderful account of this logic in the resolution by Rabbi Tobias Geffen of a problem facing the observant Jew wishing to imbibe Coca-Cola®.[43] R. Geffen inquires in 1935 of the secretive and successful Coca-Cola® company about their ingredients, a guarded formula known only to a few officials. He discovers that one ingredient (named only "M" to respect the penchant for confidentiality of the soft drink company) is made from meat and fat tallow of non-kosher animals, another ("A") is made from grain kernels, kosher but constituting leaven, therefore impermissible at Passover.

Ingredient M is there only in one part per thousand (as Geffen, properly cautious, has the chief chemist of the state of Georgia establish). No matter that that is below the halakhic admixture rate of 1:60—M nevertheless makes the beverage unacceptable, because its inclusion is intended, an act of volition.

Rabbi Geffen does not give up:

> Because Coca-Cola® has already been accepted by the general public in this country and in Canada, and because it has become an insurmountable problem to induce the great majority of Jews to refrain from partaking this drink, I have tried earnestly to find a method of permitting its usage. With the help of God, I have been able to uncover a pragmatic solution . . .[43]

He learns from some chemists that M can be replaced by a plant oil such as cottonseed oil, and A by an extract of sugar cane. Astonishingly, he convinces the Coca-Cola® company to make this substitution!

LEIBOWITZ: Most interesting in the Talmudic argument is the development of a calculus of probabilities and statistical inference. A classic case is the problem of a liquid mixture of a forbidden substance with a permitted one (e.g. milk in a meat broth; forbidden animal oil into permissible oil). If a sample is taken, can it be inferred that when actual mixing occurs, "there is homogeneity" (Hebrew: *yesh bilah*) throughout and therefore the proportions of the sample reflect exactly the proportions of the original? How large does the sample have to be with reference to homogeneity and are the rules different for liquids and solids? To learn the rabbis' solution to the problematic solution you would have to consult the Talmud.[44]

> MARY DOUGLAS: The final paradox of the search for purity is that it is an attempt to force experience into logical categories of non-contradiction. But experience is not amenable and those who make the attempt find themselves led into contradiction.
>
> *Purity and Danger*[45]

HOFFMANN: Douglas reaches for an existentialist conclusion to the question why, if dirt and pollution are nearly universally repulsive, do so many rites use unclean, impure, even abominable substances. The Lele, mentioned before, consider the anteater unclean. But they also have a cult of this animal, whose initiates touch and eat the creature.

Douglas thinks that the incorporation into human rite of absolutely everything, even the "unnatural," is inevitable. It is nature's way and so the way of societies.

It is thus evident that neither the realm of religion nor that of science is unequivocal in its stance on purity. The sacred texts of this world, despite their aspirations to purity, acknowledge the claims of inevitable, even desired admixture. And science, which first recognized the inherent tendency of the universe to mix, nevertheless strives mightily for the purity that is indispensable for a definition of impurity.[46]

V. METAPHORS THAT COMPEL

> TACITUS: For myself, I accept the view that the peoples of Germany have never contaminated themselves by intermarriage with foreigners but remain of pure blood, distinct and unlike any nation . . . Silver and gold have been denied them—whether as a sign of divine favour or of divine wrath, I cannot say . . . Even iron is not plentiful; this has been inferred from the sort of weapons they have.
>
> *Germania*[47]

HOFFMANN: Advocacy of purity seems harmless. More than that, as an inducement for the betterment of a human being in body and soul, for throwing off an idol or a drug, it serves us well. The quest for purity is normative, it describes how we *should* be. However, what gives me pause about the positive validation of purity is its abiding use by most known nationalist totalitarian movements, from fascism to apartheid.

The appeal sounded by such regimes and their propagandists is beguiling. It goes as follows: once upon a time the people were pure in body and mind, beautiful and strong. Then they were corrupted by outside forces, by foreign gods. If only the people returned to this natural pure state, if they expelled the foreign elements, if they cast out the admixture in spirit and flesh of the outsider, then, once again, the people, ah the people, would be fair and strong.

Never mind the diverse ethnic origins of Italians—such shining phrases were at the heart of Mussolini's fascist appeal. Never mind that Turks, Jews, Ukrainians, and Russians have lived among Moldavians for centuries—that's the battle cry of today's Moldavian nationalists, passing laws to keep all those others out of "their" university in Kishinev. And who marches in the vanguard of these racist, divisive forces—the intelligentsia, the religious, and the young people!

LEIBOWITZ: One must separate the legitimate from the nefarious in ethnic pride. The desire of a nation, which may be small in number, to feel it must aggressively guard its language, customs, culinary habits, and religious traditions if it is to maintain its ethnic identity (in an age when Coca-Cola is the least common denominator for all cultures) is understandable.

In Jewish law, anyone, absolutely anyone, who is willing to adopt the regimen of true observance can join the tribe. The archetypical example is Ruth, the Moabitess, mother of Davidic royalty. But a small people cannot extend the same toleration to those of its own people who want to go the other way and leave the tradition. A chemical analogy to the sweet and strong bounds of tradition might be a semiporous osmotic membrane. A barrier that permits one-way flow in, but not out.

> MICHEL TOURNIER: Purity is the malign inversion of innocence. Innocence is love of being, smiling acceptance of both celestial and earthly sustenance, ignorance of the infernal antithesis between purity and impurity. Satan has turned this spontaneous and as it were native saintliness into a caricature that resembles him and is the converse of the original. Purity is horror of life, hatred of man, morbid passion for the void. A chemically pure body has undergone barbaric treatment in order to arrive at that state, which is absolutely against nature. A man hagridden by the demon of purity sows ruin and death around him. Religious purification, political purges, preservation of racial purity—there are numerous variations on this atrocious theme, but all issue with monotonous regularity in countless crimes whose favorite instrument is fire, symbol of purity and symbol of hell.
>
> *The Ogre*[48]

HOFFMANN: It may be that the scary similarity of religious and totalitarian appeals to purity derives from their parallel rhetorical structure. The aim is to convince, with words. The situation before Mussolini or Jeremiah is the following, human one: "We are in (physical, emotional) state $\mathbf{I}$ (for impure), which I do not like. I want to exhort you to move to state $\mathbf{P}$ (for pure)." The exhortation naturally takes the form of postulating a prior state $\mathbf{P'}$ and the presence of a disturbing factor $\mathbf{X}$.

But rhetoric is not ethics, which is what got rhetoric into trouble. There is a world of difference, an ethical and spiritual essence of a difference, between fascist (or ethnic Moldavian) claims and Jeremiah. Which the parallel rhetoric, or parallel guiding metaphors, disguises.

> PRIMO LEVI: The course notes contained a detail which at first reading had escaped me, namely, that the so tender and delicate zinc, so yielding to acid which gulps it down in a single mouthful, behaves, however, in a very different fashion when it is very pure: then it obstinately resists the attack. One could draw from this two conflicting philosophical conclusions: the praise of *purity,* which protects from evil like a coat of mail; the praise of *impurity,* which gives rise to changes, in other words, to life. I discarded the first, disgustingly moralistic, and I lingered to consider the second, which I found more congenial. In order for the wheel to turn,

> for life to be lived, impurities are needed . . . Dissension, diversity, the grain of salt and mustard are needed: Fascism does not want them, forbids them, and that's why you're not a Fascist; it wants everybody to be the same, and you are not.
>
> *The Periodic Table*[49]

HOFFMANN AND LEIBOWITZ: The pure/impure dichotomy is another aspect of the central theme of man and the universe. Its other incarnations are the one and the many, the same and not the same, natural and unnatural. If there be more than one of any thing, and a way of naming or classifying each, if there is a choice, material or spiritual, the problem of purity will arise. A motion in one direction, say to segregate, inevitably raises the opposite possibility.

Two extreme arguments could be made. First, there is the line we might today call "entropic," that the natural is the most mixed. So the true path need be that of miscegenation. Support for this way could be adduced from hybrid vigor in biology. Another, contrary philosophy departs from the basic fact that the human body, in its intense local order, is inherently "contraentropic." And so we are fated to support in our thought systems and societies an opposition to mixing. To yield to disorder would be tantamount to surrendering our place in the scheme of things.

We find validity in both views and no inconsistency in a philosophy that encompasses the two. Only change is eternal. The segregated, isolated, pure, and the completely mixed impure are each in their own ways motionless and impotent. Everything else is tense, poised between pure and impure, ambiguous, therefore interesting. Alive.

NOTES

1. For most of the Bible passages we have used the new translation of *The Holy Scriptures,* Philadelphia: Jewish Publication Society, 1978. One exception is our translation of the Hebrew word *nekhoshet,* which can mean copper ore, bronze, or brass. We have followed the *Biblical Encyclopedia* in translating it as bronze everywhere except when it is clear that the context refers to copper ore in the earth.
2. Herbert C. Hoover and Lou H. Hoover in footnotes and historical notes in their translation of Georgius Agricola, *De Re Metallica* (New York: Dover Publication, 1950). See especially pp. 362, 390–93, 465–66.
3. For some leading references to ancient metallurgy see: (a) Robert Maddin ed., *The Beginning of the Use of Metals and Alloys,* Papers from the Second International Conference on the Beginning of the Use of Metals and Alloys, Zhengzhou, China, Oct. 1986 (Cambridge, Mass.: MIT Press, 1988). (b) Leslie Aitchison, *A History of Metals,* vol. 1 (New York: Interscience Publishers, 1960). (c) George Rapp, "On the Origins of Copper and Bronze Alloying," pp. 20–27 of Maddin, *op. cit.* (d) James D. Muhly, "The Beginnings of Metallurgy in the Old World," pp. 2–20 of Maddin, *op. cit.*
4. Hoover and Hoover, *op. cit.,* p. 391.

5. Biblical commentators disagree on the explanation for Jeremiah's disparagement of bronze and iron in this metaphor. For instance, Sh. D. Luzzato (19th century, Trieste) views the base metals bronze and iron as less valuable than gold and silver. On the other hand, Rashi (11th century, France) interprets the metaphor thusly: The people are slanderers strong as bronze and iron, inflicting injury upon their fellow man.

For a recent exploration of the metaphor, see Paula McNutt, *The Forging of Israel: Iron Technology, Symbolism, and Tradition in Ancient Society* (Sheffield: Almond Press, 1990).

6. Colette, *The Pure and the Impure,* translated by H. Briffault from *Ces Plaisirs* (Paris, 1932). Retitled in French in 1942 as *Le pur et l'impur* (New York: Farrar, Straus, and Giroux, 1966), p. 174.

7. In case you'd like to find out what D&C Red No. XY is, we recommend Daniel M. Marmion, *Handbook of U.S. Colorants for Foods, Drugs and Cosmetics,* 2nd ed. (New York: John Wiley, 1984).

8. Frank N. Kemmer, ed., *The NALCO Water Handbook,* 2nd ed. (New York: McGraw-Hill, 1988).

9. The meanings of pure are not exhausted by this discussion. There is a rich discourse on "pure" painting and on "pure" poetry. For poetry this may be seen in the wonderful essay by Robert Penn Warren, "Pure and Impure Poetry," in *Criticism: Foundations of Modern Literary Judgment,* edited by M. Schorer, J. Miles, G. McKenzie (New York: Harcourt, Brace and World, 1958). For art in Clement Greenberg, "Towards a New Laocoon," *Partisan Review,* July–August 1940, reprinted in John O'Brian, ed., *Clement Greenberg. The Collected Essays and Criticism. Volume I. Perceptions and Judgments 1939–1944* (Chicago: University of Chicago Press, 1986), pp. 32, 34. (The Greenberg citation comes from an interesting discussion of Anselm Kiefer's painting by Jack Flam, "The Alchemist," New York Review of Books, Feb. 13, 1992: 31–36.)

Not to speak of the senses of the word as used by (a) Mary Daly, *Pure Lust.* (Boston: Beacon Press); (b) Irwin Silverman, *Pure Types are Rare* (Westpoint, Conn.: Praeger Scientific); (c) Arthur Silverstein, *Pure Politics and Impure Science: The Swine Flu Affair* (Baltimore: Johns Hopkins University Press, 1981).

10. Matthew 5:8. The translation is from *The New English Bible* (Oxford: Oxford University Press, Cambridge University Press, 1980).

11. (a) Mary Douglas, *Purity and Danger: An Analysis of Concepts of Pollution and Taboo* (London: Ark, 1984, 54–72). See also the discussion of the Douglas thesis in Robert Alter, "A New Theory of Kashruth," *Commentary* (August 1979): 46–52; and Michael P. Carroll, "One More Time: Leviticus Revisited," in Bernhard Lang, ed., *Anthropological Approaches to the Old Testament* (Philadelphia: Fortress Press, 1985), pp. 117–26. (b) Douglas, *op. cit.,* p. 99.

12. What is particularly intriguing is that the notion about separations voiced in the blessing is intimately related to, and in fact begins with, a statement about intelligence. In explaining this, the Jerusalem Talmud asks rhetorically, "If there is not wisdom, how can there be differentiation?" This passage is inserted into the prayer for intelligence, *binah,* in the Saturday night service. Scherman, Nosson, ed. and trans, *The Complete ArtScroll Siddur* (Brooklyn: Mesorah Publ., 1984).

13. For an interesting discussion of another passage from the Prophets concerned with ritual purity, see Victor Hurowitz, "Isaiah's Impure Lips and their Purification in Light of Akkadian Sources," *Hebrew Union College Annual 60* (1989): 39–89.

14. It cannot be emphasized enough that the concept of *taharah* (purity) is one of the most complex and baffling aspects of Jewish law. The Mishnaic order of "Purities" is the longest of the six orders, and in his commentary on it, Maimonides warns that: "I wrote this introduction to disabuse you of the notion that these laws are like those of the Feast of Tabernacles, or Judges' Oaths, so that you will not read the laws of Purities and think you have grasped them on first sight . . . These are among the most abstruse of the Talmud,

being difficult even for the greatest sages. The only way to master them is to expend days and lose nights, and to progress as one accumulates penny by penny a great fortune."

15. A variety of views on the rationale for the forbidden foods are contrasted by Nehama Leibowitz, "The Dietary Laws," in *Studies in Vayikra (Leviticus)*, translated by A. Newman (Jerusalem: World Zionist Organization, 1983), pp. 76–86.
16. Wendy Doniger, "Why Should a Priest Tell You Whom to Marry? A Deconstruction of the Laws of Manu," *Bulletin of the AAAS* 44, no. 6 (March 1991): 18–31.
17. *Midrash Tanhuma, Parashat Shemini.*
18. George Frideric Handel, *The Messiah*, Section 7, Chorus, "And He Shall Purify." Other metal metaphors are used in the oratorio, in Section No. 43, Air for Tenor, based on Psalm 2:9, "Thou shalt break them with a rod of iron," and in Section No. 5 "for he is like a refiner's fire." The illustration shown is in the hand of John Christopher Smith, his principal copyist. We are grateful to Peter A. Ward Jones of the Bodleian Library for his instructive comments.
19. Nicolás Guillén, "I Declare Myself an Impure Man" (Digo que yo no soy un hombre puro), in *¡Patria y Muerte! The Great Zoo and Other Poems*, edited and translated by R. Márquez (Havana: Editorial de Arte y Literatura, 1972), 210–213.
20. (a) For an introduction to the marvels of photosynthesis, see Lubert Stryer, *Biochemistry*, 3rd ed. (New York: W. H. Freeman), chap. 22. (b) Günther Ohloff, *Perfumes and Flavors* 3 (1978): 11.
21. That there is a relentless natural tendency to disorder has been disputed, most eloquently by Ilya Prigogine. In fact, the English title of his book with Isabelle Stengers is "Order Out of Chaos." Prigogine agrees with the classical view that in closed systems (no transfer in or out of matter or energy) approaching equilibrium, entropy maximization reigns. But he and Stengers argue that in open systems, far from equilibrium, "new types of structures may originate spontaneously. In far-from-equilibrium conditions we may have transformations from disorder, from thermal chaos, into order." (Ilya Prigogine and Isabelle Stengers, *Order Out of Chaos: Man's New Dialogue with Nature* [New York: Bantam, 1988], p. 12. That is so, but only locally, over a finite period of time, and not without a disordering cost elsewhere in the universe. Prigogine's ideas are stimulating and thought-provoking. But we think they are easily overstretched, to give us what our minds desire, that order out of chaos is natural. See also the review of the Prigogine and Stengers book by Heinz R. Pagels, "Is the Irreversibility We See a Fundamental Property of Nature?" *Physics Today* (Jan. 1985): 97–99; and Rolf Landauer, "Nonlinearity, Multistability and Fluctuations. Reviewing the Reviewers," *American Journal of Physiology* 241 (1981): R107–13.
22. A most readable account of thermodynamics is to be found in Peter W. Atkins, *The Second Law* (New York: Scientific American Books), 1984.
23. Thomas Eisner, Letter [to Roald Hoffmann], 18 March 1991.
24. Of course it takes six for sex: L. B. Bjostad, C. E. Linn, J.-W. Du, W. L. Roelofs, "Identification of New Sex Pheromone Components in *Trichoplusia ni*, Predicted from Biosynthetic Precursors." *Journal of Chemical Ecology* 10, no. 9 (1984): 1309–23. Wendell Roelofs, and Thomas Glover, "Genetics of a Moth Pheromone System," chap. 9 in *Chemical Senses*, vol. 3, edited by C. J. Wysocki and M. R. Kare (New York: Marcel Dekker, 1991). Charles E. Linn, and Wendell Roelofs, "Pheromone Communication in the Moths and Its Role in the Speciation Process," to be published.
25. Robert M. Silverstein, "Pheromones: Background and Potential for Use in Insect Pest Control," *Science* 213: 1326–32, and references therein.
26. Robert L. Stevenson, *Dr. Jekyll & Mr. Hyde, the Merry Men and Other Tales* (London: J. M. Dent, 1925), p. 61. This quotation was brought to our attention by a beautiful column by David Jones, which makes some of the same points our paper does: David Jones, "Impure Thoughts," *Chemistry in Britain* 28 (1992): 928.

27. For a leading reference see Ian Baker, "Metals Pass the Endurance Test," *New Scientist,* May 30, 1992: 34–38; also J. E. Gordon, *The Science of Structures and Materials* (New York: Scientific American Library, 1988), chap. 5.
28. Samuel Noah Kramer, *The Sumerians: Their History, Culture, and Character* (University of Chicago Press, Chicago: 1963), 264–65.
29. We are grateful to Prof. Yaakov Klein of Bar-Ilan University for introducing the authors to the world of Sumer and for his thorough investigation of whether the copper in the dispute is pure copper or an alloy.

    Professor Klein personally is of the opinion that the copper, in the above disputation, represents the basic, pure copper, from which all objects, whether of pure copper or of its alloys, were manufactured. Similarly, its opponent, the silver, seems to represent all objects made from pure silver or its alloys.

    Note, however, that the term used for copper throughout this dialogue is ***urudu-kal-ga,*** copper the strong one, which may be a synonym for *zabar,* bronze. See Henri Limet, *Le Travail du Métal au Pays de Sumer,* Bibliotheque de la Faculté de Philosophie et Lettres de l'Université de Liège, vol. 155 (Paris: Les Belles Lettres, 1960).
30. Cyril Stanley Smith, "The Discovery of Carbon in Steel," chap. 2 in *A Search for Structure: Selected Essays on Science, Art, and History* (Cambridge, Mass.: MIT Press, 1981). First published in *Technology and Culture* 5: (1964): 149–75.
31. Smith, *op. cit.,* p. 35.
32. John Pettus, *Volatiles from the History of Adam and Eve* (London: T. Bassett, 1674). We are grateful to Cyril Smith for bringing this remarkable text to our attention.
33. Mircea Eliade, *The Forge and the Crucible,* translated by S. Corrin (Chicago: University of Chicago Press, 1962), p. 56.
34. Robert Hazen, "Perovskites," *Scientific American* (June 1988): 52–61. Robert J. Cava, "Superconductors beyond 1-2-3," *Scientific American* 263 (no. 2, August 1990): 42–49. R. Simon, A. Smith, *Superconductors Conquering Technology's New Frontier* (New York: Plenum, 1988).
35. Thomas Hellman Morton, Letter [to Roald Hoffmann], 12 December 1990.
36. Some excellent examples of the necessity of precisely defined mixtures are to be found in perfumery: Édouard Demole, "Parfums et Chimie: Une Symbiose Exemplaire,"*L'Actualité Chimique* (May–June 1992): 227–37.
37. This paragraph from the Jewish daily morning service originates in the Talmud, *Kritot* 6a, where the metaphor involving galbanum also appears.
38. Purity is not a simple concept. While from a physico-chemical viewpoint the incense is patently a mixture, from the ritual perspective it is "pure and holy" (Exodus 30:35).
39. According to A. Varvoglis, University of Thessaloniki, a Holy Myrrh of 57 ingredients is prepared ceremonially every decade by the Patriarchate of Constantinople, and then distributed worldwide. A 38-component version is specified in the *Mega Euchologian,* the Greek Orthodox expanded prayer book.
40. Maimonides, Introduction, chap. 6, *Commentary on the Mishnah* (in Hebrew) (Jerusalem: Mosad Harav Kook, 1978).
41. For an introduction to this subject see A. Steinsaltz, *The Essential Talmud* (New York: Basic Books, 1987), chap. 22.
42. The Delaney clause has occasioned impassioned debate since its 1958 passage. For a good introduction to its history and currency see the testimony in: United States Congress, House Committee on Government Operations, Human Resources and Intergovernmental Relations Subcommittee, *FDA's Regulation of Carcinogenic Additives* (Washington, D.C.: U.S. Government Printing Office, 1977).
43. Tobias Geffen, "A *Teshuvah* Concerning Coca-Cola," translated by Louis Geffen and M. David Geffen, in *Lev Tuviah: The Life and Works of Rabbi Tobias Geffen,* edited by Joel Ziff (Newton, Mass.: Geffen Memorial Fund, 1988), 117–21.

44. Nachum L. Rabinovitch, "Variability in Samples," in *Probability and Statistical Inference in Ancient and Medieval Jewish Literature* (Toronto: University of Toronto Press, 1973), p. 82.
45. Douglas, *op. cit.*, p. 162.
46. As might have been expected, our legal systems also struggle with the notion of purity. Does the purification of a known, patented mixture result in a product that is newly patentable? One line of legal reasoning holds that it does, another focuses on whether there is a difference "in kind" rather than "in degree" in the utility of the newer compound. See Donald S. Chisum, *Patents,* vol 1 (New York: Matthew Bender, 1978), pp. 53–57, §1.02 [9]. Also *Amgen Inc. v. Chugai Pharmaceutical Co. Ltd.,* 13 U.S.P.Q. 2d 1737, 1759 (D. Mass. 1989). We are grateful to C. Frederick Leydig for bringing these cases to our attention.
47. Tacitus. "Germania," 4–6, translated by H. Mattingly (Hammondsworth: Penguin, 1970), 104–105.
48. Michel Tournier, *The Ogre,* translated by Barbara Bray (Garden City: Doubleday, 1972), p. 75. The French original is entitled *Le Roi des Aulnes* (Paris: Gallimard, 1970), p. 85.
49. Primo Levi, *The Periodic Table,* translated by R. Rosenthal (New York: Schocken, 1984), 33–34.

Acknowledgment: Many friends and colleagues made useful comments on drafts of this contribution, or pointed us toward important references. We thank Herbert Deinert, Thomas Eisner, Hillel Furstenberg, Yaakov Klein, C. Frederick Leydig, Thomas Morton, David Owen, Wendell Roelofs, Elizabeth Sherman, Cyril Stanley Smith for their help.

FIRENZE - Museo di S. Marco
Beato Angelico
Madonna della Stella (Tabernacolo)
Vierge de l'étoile (Tabernacle)
Virgin of the star (Tabernacle)
Jungfrau des Sternes (Tabernakel)

NOVA LVX

1124 C

Dear Alfred,

Thanks for the books, yours and Wischnitzer's. I already found an important article, on the sotah, or ordeal of bitter waters, in it.

I wonder what is the foreground right object in your painting. Perhaps it's a case for arrows. If so what is its iconographic significance. I'll have to go back and read the Bible.

9/25/95 Rosh Hashana Regards. Paola
Happy New Year

Ediz. Giust. 8 ...
da Fotocolor Kodak Ektachrome
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Non scrivere al di sotto di questa riga Do not write below this line Ne pas écrire au dessous de cette ligne Bitte nicht unterhalb dieser linie schreiben No escribir debajo de esta raya

OK SPEDISCI QUALITÀ

ALFRED BADER FINE ARTS

DR. ALFRED BADER

ESTABLISHED 1961

October 16, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

I am sorry that my traveling a good deal has delayed my responding to your question about the painting on the cover of my book.

A full reproduction of that is enclosed. I am not certain whether the man is a medical man or a chemist, but I don't think that the story is Biblical.

With all good wishes, I remain,

Yours sincerely,

AB/cw

By Appointment Only
ASTOR HOTEL SUITE 622
924 EAST JUNEAU AVENUE
MILWAUKEE WISCONSIN USA 53202
TEL 414 277-0730 FAX 414 277-0709

from "The Same and Not the Same"

Roald Hoffmann

FRITZ HABER

The creative chemist is moved by the problem at hand, and general curiosity about the molecular world. Material support from society is certainly needed. For that support the chemist offers his or her energies in the advancement of reliable knowledge, once in a while even something practical. Who can blame him for wanting to be left alone most of the time; recalcitrant and beautiful matter presents enough problems of its own.

But this is not the way it is. The world has its ways of impinging on the creative scholarly life, of engulfing the person. The chemist would like the world to leave him alone; it has its own ways of touching him, in the beginning, in the middle in the end of life. In no case that I know has this scenario been played out with more drama then in the life of one of the greatest of all physical chemists, Fritz Haber.[1]

Haber was born in German Silesia in 1868, the son of a prosperous German Jewish merchant. Early in life he converted to Christianity, a fairly typical tactic of assimilated upward-mobile Jews in Europe in the early part of the nineteenth century. By Haber's time conversion was not necessary to achieve high status in the academic world — Richard Willstätter, one of this century's great organic chemists, did not feel the necessity for conversion. Nor did Albert Einstein. Haber did; while he surrounded himself with Jews and people of Jewish ancestry throughout his life, he wore a convert's mask until close to the

end of his life.

Haber's early years were marked by struggles with his father (his mother died days after his birth). Interestingly, one of these involved a difference of opinion on the commercial role of synthetic dyes, the centerpiece of the then developing German fine chemical industry.

As much as Haber may have resented the early commercial exposure, perhaps it was the source of a unique talent that he showed later in life, for blending pure and applied science. One of his students, Karl Friedrich Bonhoeffer, later wrote of Haber.

> Free of all academic narrowness, he cherished in his work the close reciprocal relationship of technology and pure science. In this way he developed into a scientific personality whose intellectual concern was always devoted to preserving the ties between scientific progress and practical life.[2]

Haber did not have a great mentor. Nor did he begin his scientific career with a stellar success, a great synthesis, the discovery of some great law of nature. Instead he labored largely by himself, on diverse problems in organic and physical chemistry. Throughout his life Haber had a tremendous capacity for work, and for assimilating the new. Fritz Stern, a thoughtful observer of the German historical and intellectual scene, makes the following point:

> From childhood on, Haber lived in historically dramatic times. His formative years coincided with the exaltation occasioned by Germany's unification, that belated achievement which gave the Reich its fatal militaristic-authoritarian character that even Bismarck at times regretted...It would be foolish to draw too close a parallel between the development of the nation

> and young Haber, but the triumphs of both had something to do with feelings of inferiority which so many Germans wanted to exorcise. How many Germans transported their feelings of discontent of whatever origin in ceaseless work![3]

Haber's greatest achievement was the ammonia synthesis which I mentioned in the last chapter. It arose from complete understanding of the constraints of chemical equilibrium; what's interesting is that Haber was self-taught in physical chemistry. The eventual success also owes much to a determination, a stubbornness, which is perhaps exemplified by this story, which according to Morris Goran, Haber told about himself:

> One very warm summer day he went hiking in the Swiss mountains. After a jaunt of eight hours, searching for drinking water, he came to a very small, seemingly uninhabited place. Water was not to be found, and he was very thirsty. Finally, he saw a well surrounded by a low wall. He immediately immersed his entire head. At almost the same time and unnoticed by him, a bull had done likewise; neither paid much attention to the other. But when they withdrew from the water, they found their heads had been interchanged. Fritz Haber had a bull's head and prospered as a professor from the eventful day.[4]

At the beginning of the ammonia story is a failure, and in its middle lies a scientific controversy, both of which only spurred Haber on.

Many had worked on the ammonia synthesis. In 1904 two Viennese entrepreneurs, the Margulies brothers, approached Haber to work on making ammonia from the elements. Haber and his students tried several metals, hoping to convert the N_2 to a

metal nitride, which would then go on to react with H_2. But the temperatures needed were so high that little ammonia formed. The financial support from the sponsors dried up; the project seemed to be lost.

The failure rankled. Worse was to come in a questioning of Haber's data on the ammonia equilibrium by Walter Nernst, the dean of German thermodynamics. The point at question was the actual ratio of N_2, H_2 and NH_3 at equilibrium. Nernst had also worked on the ammonia synthesis at higher pressures. His theoretical understanding of what was necessary to achieve an effective synthesis was not inferior to Haber's. But Nernst had obtained a value of the so called "equilibrium constant" of the reaction

$$N_2 + 3H_2 \rightleftarrows 2NH_3$$

that indicated there would be less ammonia present at equilibrium than Haber had measured. Sufficiently less so that commercial synthesis was unlikely.

Haber and Nernst had clashed before, and were to do so again. In this case Haber took Nernst's experiments, done at higher pressures, as a challenge. Together with Robert Le Rossignol, he redid his experiments with great care, and showed that Nernst was wrong.

More importantly, the controversy focused Haber's energies on the effect of pressure. Recall that the ammonia side of the

equilibrium has two molecules, not four, as on the nitrogen plus hydrogen side. So an increase in pressure would favor the side of smaller volume (less molecules). This is the way to make more ammonia. Except that the pressures required exceeded those used in the chemical reactors (glass and metal vessels) in use at the time. Haber and his coworkers, including a skilled metal worker, Kirchenbauer, developed the containers and the methods of achieving the requisite high pressure, as well as the osmium and uranium (nothing to do with radioactivity) catalysts needed to help the reaction go at low temperatures.

Perhaps never before had a laboratory process for an industrial reaction been developed as thoroughly in an academic setting. Haber was fortunate in the sequel, in that the engineer who took over the process at BASF, then and now one of the world's great chemical companies, was the talented and ingenious Carl Bosch. Bosch developed a less expensive catalyst and transformed the reaction into an effective industrial synthesis. The Haber-Bosch process, perfected in small ways, is still in use today for the synthesis of most of those 3.6×10^{10} lbs. of NH_3.[5]

In my view, there is no doubt that Haber's achievement was and is a boon to humanity. The major use of ammonia is as a fertilizer; this in fact is the primary use of most of the chemicals produced in high volume in the world. This century has

Illustration 65 here: Portrait of Fritz Haber.

witnessed an incredible population explosion. Chemically intensive modern agriculture has managed to feed adequately (on the average, not without local famine) all those additional mouths. The yield from a good American acre of corn (150 bushels) is up by a factor of six since 1800. There is a case to be made for "organic" agriculture, but I think that synthetic fertilizers, and Haber's invention in particular, have prevented the starvation of hundreds of millions of human beings.

The Haber-Bosch process came on stream just in time for Germany. With the outbreak of war in 1914, the German supply lines to South American fertilizer sources were cut. And most munitions contain much nitrogen, from TNT (trinitrotoluene) to ammonium nitrate (a fertilizer and an explosive used in the 1993 World Trade Center bombing). There were other industrial sources of nitrogen—containing compounds — coal distillation and the cyanamid process — but it can be argued that Haber's discovery was critical. What was a way of "making bread out of air", was also essential to the war.

During the war Haber put the ingenuity and talent of his institute and his personal energies into the development of "chemical" weapons. I put the descriptor in quotation marks to point out the absurdity of the differentiation — as if gunpowder, metal, explosives were not chemical! The Hague convention had outlawed "poison or poisoned weapons". There was some limited activity on both sides of the conflict prior to the war, but as L.F. Haber, who has written the definitive study of chemical

warfare in World War I (and who is Haber's son), says

> The most one can say about gas and smoke is that by the eve of the war military awareness of chemicals had increased to the extent that some soldiers were willing to consider them and a very few, with a more innovating turn of mind, were even experimenting with various compounds. The substances used with the exception of phosgene, were not toxic. There were no military stocks of gases, nor of gas shell, save for very limited supplies of tear-gas grenades and cartridges in French hands. The forerunners were scientific curiosities and the belligerents of August 1914 had no conception of the practicalities of chemical warfare.[6]

They acquired them quickly. Haber's contribution was the concept of a gas cloud, his choice of chlorine and other chemicals, and his continued dedication. The German supreme command found in Haber "a brilliant mind and an extremely energetic organizer, determined, and possibly also unscrupulous."[7] He left decisions as to the legality of the use of poison gas to the high command.

Here is a description of the first large-scale gas attack, at Ypres, on the afternoon of April 22, 1915.

> The simultaneous opening of almost 6,000 cylinders which released 150 t of chlorine along 7000m within about ten minutes was spectacular. The front lines were often very close, at one point only 50 m apart. The cloud advanced slowly, moving at about 0.5 m/sec (just over 1 mph). It was white at first, owing to the condensation of the moisture in the surrounding air and, as the volume increased, it turned yellow-green. The chlorine rose quickly to a height of 10-30 m because of the ground temperature, and while diffusion weakened the effectiveness by thinning out the gas it enhanced the physical and psychological shock. Within minutes the Franco-Algerian soldiers in the front and

> support lines were engulfed and choking. Those who were not suffocating from spasms broke and ran, but the gas followed. The front collapsed.[8]

Men died in so many ways in this war, as in other wars. This was a new way. It was not an exclusively German way of killing, for the chemistry was in the end simple and smart men and industry were there on both sides. Chlorine, phosgene, mustard gas, chloropicrin were used extensively by Germany's opponents as well. Nor did poison gases just kill. Many more soldiers were injured, some badly, L.F. Haber estimates deaths as 6.6% of all gas casualties.[9]

Rationalizers of gas warfare, then and now, ask "Is there a nice, good way to die? What is worse about poison gas than shrapnel?" The answer is to be found in the testimony of the wounded. Something in the psyche, something deep that associates life with breath, is perturbed. Here is a section from Wilfred Owen's poem "Dulce et Decorum Est":

> Gas! Gas! Quick, boys!——An ecstasy of fumbling,
> Fitting the clumsy helmets just in time;
> But someone still was yelling out and stumbling
> And flound'ring like a man in fire or lime...
> Dim, through the misty panes and thick green light,
> As under a green sea, I saw him drowning.
>
> In all my dreams, before my helpless sight,
> He plunges at me, guttering, choking, drowning.
>
> If in some smothering dreams you too could pace
> Behind the wagon that we flung him in,
> And watch the white eyes writhing in his face,
> His hanging face, like a devil's sick of sin;
> If you could hear, at every jolt, the blood
> Come gargling from the froth-corrupted lungs,
> Obscene as cancer, bitter as the cud

Of vile, incurable sores on innocent tongues,–
My friend, you would not tell with such high zest
To children ardent for some desperate glory,
The old Lie: Dulce et decorum est
Pro patria mori.[10]

The number of gas casualties to all combatants was relatively small, 3 to 3.5% by L.F. Haber's well-reasoned estimate.[11] The weather — wind, rain, heat — prevented then and still does, the effective tactical use of chemical weapons in warfare. But the psychological stain of this weapon is indelible.[12]

I wonder if Haber, so experienced in catalysis, thought of poison gas (or of himself) as a catalyst, intended to speed up the outcome, to end the bloody stalemate of trench warfare. This was not to be. Germany lost the war. And another casualty was Haber's wife Clara, a chemist herself. She pleaded with her husband to give up his work on chemical weapons. He refused. We cannot know the causal connection, but she committed suicide.

After the war, Germany was saddled with a tremendous reparations debt of 33 billion dollars, much of it payable in gold. Haber, now the recipient of a Nobel Prize for the ammonia synthesis, the leader of German chemistry, set his sights on extracting gold from sea water. He translated the total war debt into the equivalent of 50,000 tons of gold. The oceans were estimated by an Australian chemist, Archibald Liversidge, to contain 30 to 65 milligrams of gold per ton of sea water. This translated to 75 to 100 billion tons of gold in the oceans. The North Sea alone would do to the settle Germany's debt.

Haber did a series of experiments on "synthetic sea water", precipitating the gold ions with lead acetate and ammonium sulfide. He came to a conclusion that the gold could be economically separated if its abundance were even as low as 5mg per ton of sea water. He then set about to check the previous literature estimates of gold concentrations, even equipping in high secrecy a Hamburg-American Line ship with a laboratory and extraction plant.

Haber was now in the business of analysis, which we have seen is an art and a science. Here is an account of what happened:

> Gradually however, problems arose. Haber covered vast areas of the Atlantic, and the water of Iceland and Greenland as well as the North Sea. He found the presence of gold varied considerably by region—for example, ten times as much gold appeared for a given volume in the North Atlantic as in the South Atlantic. Taking over 100 samples from offshore waters near the Californian gold fields, he found that even tidal changes made a great difference in results. Moreover, it appeared that when methods satisfactory for high concentrations were used with waters containing low concentrations, the results reflected the presence of gold in the reagents and vessels used...Eventually, Haber decided that Liversidge was simply wrong; and on two points disagreed with him: gold nowhere exceeded .001 mg/m^3; and occurred with suspended matter rather than in solution.[13]

We come here to another tension characteristic of chemistry — suspicion and trust. Haber believed Liversidge's earlier analysis, as well as that of Sonstadt, another chemist active in this field. In the papers he subsequently wrote

> Haber divided his criticism between Sonstadt, who had undoubtedly been deceived by reagent contamination, and who in an article published in 1892, seemed to admit as much; and Liversidge, whom he faulted on technical grounds. Liversidge had used a method which required extremely sensitive methods of extraction. Sadly, in Haber's words "diese Vertrautheit hat Liversidge nicht besessen". Liversidge had simply produced results using unsatisfactory procedures.

The modern alchemist was disappointed.

In early 1933 Hitler and the National Socialists came to power, with their baggage of antisemitic views. Already in April of that year they issued a decree for purging Jews from the civil service. Haber's world broke apart; he, who was not really a Jew, now was a Jew. Haber had represented one pole of German Jewry; not only completely integrated into German culture, but patriotic in the extreme. Albert Einstein represented another pole — German, but always suspicious of his native country. Haber was crushed by the events, morally despondent. Fritz Stern describes the situation:

> ...the silence of colleagues, the betrayal by the elites, was devastating. From exile, Einstein wrote Haber a letter full of compassion for his fate: "I can imagine your inner conflict. It is as if one must give up a theory which one has worked on all one's life. it is not the same for me because I never believed in it in the least." The theory was faith in German decency, in a future in which Jews and Christians could live and work together.[14]

Haber could have stayed on in his position since the law for the moment excluded war veterans from dismissal. He would have been forced, however, to dismiss his Jewish coworkers. Instead

he resigned. This is an excerpt of his letter of resignation of April 30, 1933 to the Nazi Minister of Science, Art and Education:

> My decision to request my retirement follows from the contrast of the research tradition in which I have hitherto lived with the different views which you, Mr. Minister, and your Ministry advocate as protagonists of the present great national movement. In my scientific office my tradition demands that in choosing my collaborators I take into account only the professional and personal qualifications of applicants without regard to their racial background. You will not expect a man in the sixty-fifth year of his life to alter a way of thinking which has guided him for the past thirty-nine years of his university life, and you will understand that the pride with which he has served his German homeland all his life now dictates this request for retirement.[15]

The minister said he was well rid of the Jew Haber. Now there was no mask; Haber wrote to Einstein in August 1933 "In my whole life I have never been so Jewish as now".[16] Fritz Jakob Haber left Germany for Switzerland, thought about a position in the country of his former enemies, England, thought about settling in Palestine. He was a broken man; this great German chemist died on January 29, 1934 in Basel, geographically close to his homeland, spiritually very far removed indeed.

Less than ten years later, another product of the chemical industry, another gas, was used in the murder of millions of Haber's people in the extermination camps.

1. The definitive biography of Haber has just been published in German: Dietrich Stoltzenberg, Fritz Haber: Chemiker, Nobelpreisträger, Deutscher, Jude, (Weinheim: VCH, 1994). I am grateful to Peter Gölitz for making available to me a section of this biography prior to its publication. There is an earlier biography by Morris Goran, The Story of Fritz Haber, (Norman: University of Oklahoma Press, 1967), and a novel on his life, Herman Heinz Wille, Der Januskopf, (Berlin: Buch Club 65, 1970). There is also a chapter in Richard Willstätter's autobiography From My Life, (New York: W.A. Benjamin, 1965). Haber's scientific work is beautifully reviewed in a memorial lecture, J.E. Coates, J. Chem. Soc. (1939) 1645.

A most perceptive analysis of the life of this great chemist, ably set in his tumultuous times, is the chapter by his godson and outstanding scholar of European history, Fritz Stern, Dreams and Delusions, (New York: Alfred A. Knopf, 1987), p. 51-76.

2. Karl Friedrich Bonhoeffer, Chemiker Zeitung 58, (1934). Stern, Dreams and Delusions, p. 294 remarks "It was an act of courage [in 1934] to publish an obituary about a Jewish chemist, an act characteristic of Bonhoeffer and of his entire family, which behaved so heroically and suffered so cruelly under the Nazis."

3. Stern, Dreams and Delusions, p. 55, 6.

4. Goran, Dreams and Delusions, p. 23.

5. For further information on Karl Bosch, see George B. Kauffman "Two High-Pressure Nobelists," Today's Chemist, **3**(4), (1990).

6. L.F. Haber The Poisonous Cloud, Clarendon Press, (Oxford: 1986), p.

7. Haber, The Poisonous Cloud, p. 27.

8. Haber, The Poisonous Cloud, p. 34.

9. Haber, The Poisonous Cloud, p. 244.

10. Wilfred Owen, "Dulce et Decorum Est", in Alexander W. Allison et al, eds. The Norton Anthology of Poetry, 3rd Ed. (New York: W.W. Norton, 1983), p. 1037.

11. Haber, The Poisonous Cloud, p. 242.

12. An interesting point raised by Mary Reppy is that chemists do not seem to have the deep feelings of guilt or responsibility about the development of "chemical" warfare that (some) physicists have about the atomic bomb. Why? Reppy mentions three possibilities: (1) that chemical weapons were used earlier (and so we have had time to forget...); (2) chemical weapons are nominally outlawed; (3) the development of poison gases did not become "the boon/shaping moment" for chemistry the way the

Manhattan Project was for physics. (M. Reppy, private communication).

13. R.M. MacLeod, "Gold from the Sea: Archibald Liversidge, F.R.S., and the "Chemical Prospectors"; 1870-1970," Ambix 35(2) (1988): 53-64.

14. Stern, Dreams and Delusions, p. 73. The Einstein quotation is to a letter by Einstein to Haber of 19 May 1933, Einstein Papers, Boston.

15. Cited in full in Willstätter, From My Life, p. 289.

16. Stern, Dreams and Delusions, p. 74, citing a letter in the Max Planck archive.

Dr. Alfred Bader
2961 North Shepard Avenue
Milwaukee, Wisconsin 53211

A Chemist Helping Chemists

September 18, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

Thank you so much for sending me the order form for your book, *The Same and Not the Same*. I hope you won't mind that I send the check to you in the hope that you will send me an inscribed book.

America's greatest art historian - both in competence and humanity - in the middle of this century was Wolfgang Stechow at Oberlin. You might not know his paper on the depiction of Jacob blessing his grandchildren, and so I enclose a copy.

Just recently I was able to purchase a small painting of that subject at Christie's in London, except they had offered as "Isaac Blessing Jacob"!

We haven't seen you for the longest time; couldn't you come to Milwaukee and see hundreds of new acquisitions?

With all good wishes from house to house, as always,

AB/cw

Enclosures - 2 books, check, Xerox copies

Dr. Alfred Bader
2961 North Shepard Avenue
Milwaukee, Wisconsin 53211

A Chemist Helping Chemists

October 3, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

I am so enjoying reading your book.

Enclosed please find a complete reproduction of the painting on the cover of my autobiography. Of course, I am not certain whether the old man is an alchemist or a medical man. I particularly like the four, so different light sources. I don't think that this is a Biblical painting.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Enclosure

Dr. Alfred Bader
2961 North Shepard Avenue
Milwaukee, Wisconsin 53211

A Chemist Helping Chemists

September 13, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

Just a note to tell you how very much I enjoyed reading the draft of your chapter, "You shall not deviate to the left and to the right".

For some years now, our congregation here in Milwaukee has asked me to say a few words on Yom Kippur, in the afternoon service after the reading of the Book of Jonah. This year I will be guided by your chapter and speak about the very last words in the Book of Jonah.

Just two suggestions:

On page 11, in the first quotation, Rabban Gamliel sent to Rabbi Joshua.

On page 27, after the quotation, "It is not in heaven," you might like to add the entire passage from Deuteronomy <u>30</u>, 12, to show where this comes from.

I have never seen an essay that combines such good chemistry with Talmudic commentary.

Where and when will this be published? I can hardly wait to read the entire book.

I really appreciate your permission to use the excerpt from Bob Woodward's Cope lecture relating to Couper.

What a pity that Bob didn't know about Loschmidt. I would have loved to hear his comments about both my essays; copy of that on Loschmidt is enclosed. Both will be published by Plenum.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Enclosure

Dr. Alfred Bader
2961 North Shepard Avenue
Milwaukee, Wisconsin 53211

A Chemist Helping Chemists

September 6, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Baker Laboratory
Ithaca, NY 14853-1301

Dear Roald:

Thank you for your postcard and that wonderful draft entitled "You shall not deviate to the left and to the right." How big will the entire book be, and where will it be published? You also mentioned in your postcard that you were attaching "an ad for an absolutely great book", but that was not included.

Thank you for citing my "Bible Through Dutch Eyes"; you will have noted that I included quite a few Talmudic references in that.

Thank you also for allowing me to quote from Bob Woodward's Cope lecture. I first heard about Couper from Bob in the late 1940's and now enclose a rough draft of my paper to be published by Plenum with the other Loschmidt talks. I also enclose a copy of the program and just wish that you could have been there.

I have only had a chance to read through that wonderful draft about chirality and the Bible once, but I would like to read it several times and then write to you again.

Incidentally, a curator friend once explained to me how I can tell which of two very similar paintings is the original and which the copy. Look at each in the mirror. The original will look right, and the copy will not.

With fond regards, as always,

AB/cw

Enclosures

Dr. Alfred Bader
2961 North Shepard Avenue
Milwaukee, Wisconsin 53211

A Chemist Helping Chemists

August 21, 1995

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Ithaca, NY 14853-1301

Dear Roald:

It was kind of you to permit me to use an excerpt from Bob Woodward's Cope lecture in my future talks on Couper.

In June, there was a Loschmidt Symposium in Vienna, and I enclose part of the program.

In my second talk, relating to Anschütz, Couper and Loschmidt, I related that I had first heard about Couper from Bob Woodward in informal discussions while I was a student at Harvard and then in the Cope lecture in Chicago. However, as I didn't have the Cope lecture in Vienna, I could only refer to it.

Plenum is planning to publish the text relating to all the lectures given, and I enclose my proposed text for my talk. Do you think I am right in actually quoting Bob's lecture, rather than just referring to it? Of course, I could easily take out the actual quotation and just paraphrase it briefly, as I did in Vienna. But actually, the full quotation adds so much to the paper, and I would very much like to have your and Ted's opinions as to whether you think the full quotation is appropriate.

We haven't seen you for the longest time and hope that you will have a chance to come to Milwaukee before long.

With all good wishes from house to house, I remain,

Yours sincerely,

AB/cw
Enclosures
cc: Dr. Theodor Benfey

COLLÈGE DE FRANCE
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J.-M. LEHN, Professeur

Written from Paris,
but mailed from Ithaca

RECEIVED
6-4-84

5 4

May 18, 1984

Dear Al: ← I'm not sure this is right. So apologies if it isn't

I'm spending a month with Jean-Marie Lehn here, at the end of a leave. Here is a painting I saw in De Jonckheere's gallery in Paris. It's by Jan Griffier, Amsterdam 1652–London 1718, "Paysage Vallonée", 23.5 x 29.5cm. I like portraits better, but this one caught my eye because of a very nice treatment of the bright light coming from behind the outcrop at center, and the details of the mountain landscape.

Do you know anything about Griffier? I could do some research, but I thought I would turn to the expert first. They want 135,000 francs, or ~$16,000 for it.

Regards
Roald

Please return the photo eventually since I promised it back to them.
I will be here until June 14, then traveling in Europe, so its best to write to Ithaca after ~June 5.

File
R. Hoffmann

OCKHAM'S RAZOR AND CHEMISTRY

by

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Summary: We begin by tracing the personal and scholarly history of William of Ockham, the man whose name Ockham's Razor (OR) bears. His various formulations of the principle of parsimony are presented. We then define a reaction mechanism and tell a personal story of how OR entered the study of one such mechanism. A small history of methodologies related to OR, least action and least motion, follows. This is all done in the context of the chemical (and scientific) community's almost unthinking acceptance of the principle as heuristically valuable. Which is not matched, to put it mildly, by current philosophical attitudes toward Ockham's Razor. What ensues is a dialogue, pro and con. We first present a context for questioning, within chemistry, the fundamental assumption that underlies OR, namely that the world is simple. Then we argue that in more than one pragmatic way OR proves useful, without at all assuming a simple world. OR is an operating manual, not a world view. Continuing the argument we look at the multiplicity and continuity of concerted reaction mechanisms, and at principal component and Bayesian analysis (two ways in which OR is embedded into modern statistics). The dangers to the chemical imagination from a rigid adherence to an OR perspective, and the benefits of the use of this venerable and practical principle are given, we hope, their due.

[a] Cornell University

[b] Rostov-on-Don University

Scientists think they are born with logic; God forbid they should study this discipline with a history of more than two and a half millenia. Isn't it curious that some of their competitors and critics seem to be strangely deficient in logic!

While scientists think they can do without philosophy, occasionally principles of logic or philosophy do enter scientific discourse explicitly. One of these philosophic notions is Ockham's Razor (OR), generally taken to mean that one should not complicate explanations when simple ones will suffice.

The context in which OR is used in chemistry is either that of argumentation (trying to distinguish between the quality of hypotheses) or of rhetoric (deprecating the argument of someone else). Either way, we think that today appeal to OR has a bit of a feeling of showing off, of erudition adduced for the rhetorical purposes. This attitude reveals a double ambiguity. The first is toward learning —— today's science, no longer elitist, does not depend on men steeped in classical learning. And appeal to OR also points to a certain ambiguity in the relationship of science to philosophy.

We thought it would be interesting for chemists to learn something of the man whose name the principle bears, and its various meanings. We also present a personal discussion on the use of OR in science, with specific reference to the analysis of reaction mechanisms.

WILLIAM OF OCKHAM

Scientists think they can avoid the politics of their times. They can't. Neither could medieval theologians and philosophers, one of whom was William of Ockham (or Occam). We know precious little of his early life.[1] He was born in the village of Ockham in Surrey near London, probably within five years of 1285. The first certain date we have in his life is February 26, 1306 when he is ordained subdeacon of Southwork. William entered the Franciscan order, tremendously popular at that time, at an early age. He is likely to have studied at Oxford from 1309 to 1315, and continued his philosophical work there and in London from 1315-1324. Despite the tremendous quantity and quality of his scholarly work in this period (the so far incomplete definitive edition of his work, being published by the Franciscan Institute at St. Bonaventure, NY, and by Manchester University Press, runs to nine volumes of theology, six of philosophy and two of politics[2]) he never held a chair at Oxford. This was due to the enmity of the Chancellor of Oxford at the time, John Lutterell, who has been characterized as "an overzealous Thomist",[3] a nasty character by all accounts.

In 1324, William's life changes. The politics of the various orders of the Catholic Church, and the interplay of secular and religious power in this period are most intricate. Perhaps reading the section of Umberto Eco's <u>The name of the rose</u> that most readers skipped might help.[4] The papacy in this time is buffeted by secular power struggles, and resides in exile in Avignon, France (from 1309-1377). John Lutterell travels there in 1323, to Pope John XXII, accusing William of Ockham of fifty six instances of teaching dangerous doctrine. Ockham is summoned to Avignon in 1324, and a commission is appointed to examine his teaching. Essentially this was a trial for heresy. It dragged on for three years, and never reached a formal conclusion as other events overtook it.

The Franciscans were at this time involved in dispute with the Pope, an argument with the usual mix of theological and financial overtones. The theoretical side concerned the question whether Christ and the Apostles possessed property in private or in common. Behind this discussion lay the issue of the ideal of poverty, favored by some orders, and opposed by others. Even within the Franciscan order there was substantial division on whether the community of friars had to follow the path of poverty that individual friars did. The General of the Franciscan order, Michael of Cesena, asked William of Ockham to study the issue. William's intellectual honesty and depth of logic led him past simple disagreement with the Pope on this issue. He found many of John XXII's statements contradicting earlier authority, and he said so. Eventually, in 1328, William joined his General and two other Franciscans in defying the Pope. They fled to Pisa, and there obtained the protection of the German Emperor, Ludwig (Louis) of Bavaria. Ludwig had his own political agenda; he had installed an Anti-Pope in Rome, and had himself crowned as Emperor of the Holy Roman Empire.

So began the period of the rival papacies and 20 years of mostly political activity for William of Ockham. Excommunicated by the Avignon Pope, the rebellious Franciscans settled at the court of Ludwig in Munich. Upon the death of their protector in 1347, their position became untenable. William sent back to Avignon the seal of the order, which he held, and a document of submission was drawn up. It was never signed; William died, probably a victim of the Black Death, c. 1349.

THE THEOLOGIAN AND PHILOSOPHER

William of Ockham may be known to chemists as the man whose name is associated with OR. To his peers and to the world of theology he was and is a leading "scholastic" philosopher. This is the end of the Middle Ages; the wisdom of the Greeks is reintroduced into Europe through Al Andalus, Islamic Spain. It is a time of great minds in the religions; the time of the Rabbis Moses ben Maimon (Maimonides) in Cordova, Moses ben Nachman (Nachmanides) in Gerona, Shlomo Yitzhaki (Rashi) in Troyes. It is the time, or shortly after the time, of St. Thomas Aquinas, of Roger Bacon, of Duns Scotus. The philosophy of Aristotle, with its far-reaching rationality, finds a resonance in the agile minds of Catholic theologians. The glory of God merges in their work with the path of reason; there is no disjunction between faith and rationality for these men.

A basic principle of William of Ockham's theology is that all things are possible for God, save such as involve contradiction. So we may learn more of our (His) religion by probing its logical depths. In some ways this is an early statement of the philosophical rationale that produced (much later) the religious scholar-students of nature, especially the great scientists of the Jesuit order.

It becomes important (for William and his scholastic contemporaries) to seek out contradictions, to probe causes, to seek the reason for all but the First Cause. That search may seem to us abstruse. As in this typical passage:

> ...Sudden change is not a thing (res) distinct from permanent things and destroyed after the first instant at which the subject is suddenly changed...Rather for the subject to change suddenly is only for the subject to have a form that it did not have earlier or lack a form that it had earlier——nevertheless, not part by part in such a way that it has one part of the form before the other; nor does it lack one part before it lacks another. But it receives the whole form simultaneously or loses the whole simultaneously.[5]

Perhaps a brake on calling a passage such as this "abstruse" might be the reflection on how a typical paragraph from one of our papers might sound to a scholastic philosopher, or for that matter to any intelligent human being who is not a chemist. Interestingly, an astute observer, Mary Reppy, remarks that the last part of this passage sounds awfully like an attempt to define a concerted reaction.[6] Of which more, anon.

THE RAZOR

William of Ockham was not only a theologian, but a great logician. A case has been made for his awareness of many of the principles of mathematical logic that were not mathematicized until 600 years later.[7] One of the tools he used routinely in his reasoning is what is known in philosophy as the principle of parsimony, and popularly as Ockham's Razor.

Just as for the Golden Rule, there are many ways of stating OR. Here are four that William of Ockham used in his works:[8]

> (A) It is futile to do with more what can be done with fewer. ["Frustra fit per plura quod potest fieri per pauciora".]
>
> (B) When a proposition comes out true for things, if two things suffice for its truth, it is superfluous to assume a third. ["Quando propositio verificatur pro rebus, si duae res sufficiunt ad eius veritatem, superfluum est ponere tertiam."]
>
> (C) Plurality should not be assumed without necessity. ["Pluralitas non est ponenda sine necessitate."]
>
> (D) No plurality should be assumed unless it can be proved (a) by reason, or (b) by experience, or (c) by some infallible authority. ["Nulla pluralitas est ponenda nisi per rationem vel experientiam vel auctoritatem illius, qui non potest falli nec errare, potest convinci."]

Philosophers and historians are generally puzzled as to why the principle of parsimony should be called Ockham's Razor. The principle is not original to William of Ockham. Versions of it are to be found in Aristotle, and nearly *verbatim* variants occur in the work of most scholastic philosophers.[9,10] Though Ockham used it repeatedly and judiciously, "he clearly does not regard it as his principal weapon in the fight against ontological proliferation".[11]

We suspect that the association is due to the strength of the razor metaphor rather than anything else. Scholastic and theological arguments were complex; to cut through them, to reach the remaining core of truth quickly, was desperately desirable. Whoever rechristened the principle of parsimony as Ockham's *Razor* (the earliest reference appears to be to Condillac in 1746[12]) was creating an easily imagined image. Metaphor reaches right into the soul. As much as scientists would like to deny the power of metaphor...

The last, most extensive formulation of OR, (D) above, is intriguing. Note the "religious exclusion" in part (c). It refers to the Bible, the Saints and certain pronouncements of the Church. This testimony to the faith of William did not stop him from questioning the infallibility of Pope John XXII, when the Pope's writings came in conflict with earlier church authority. In the context of science, especially interesting is (b), that experience ("experientiam") can serve to justify plurality. There is no reason not think of "experience" here as "experiment", even though the idea of a scientific experiment lies centuries in the future. William of Ockham's method (and that of Aristotle) empowers the human senses as arbiters. His method accepts what we now call science.

REACTION MECHANISMS

Six and a half centuries is a lot of time; it is also very little time. In the Middle Ages one had protochemistries —— fermentation, metallurgy, ceramics, alchemy, dyeing. People have always transformed matter in ingenious ways. The Renaissance came, then the Industrial and Scientific Revolutions. Now there is chemistry, a true science, an industrial empire, a profession. Beautiful molecules are made, fifteen million of them unknown to Nature. People ask questions "How does this reaction run?" "What is the mechanism (a very Newtonian clock-work type of question) of that reaction?" And remarkably, six hundred and fifty years after he died, they invoke William of Ockham's restatement of the principle of parsimony, that old Ockham's Razor, to help them reason out what happens.

Let us first define what is to be meant by the term "reaction mechanism". The notion of the mechanism of a chemical reaction consists of a description of all "elementary" steps in the transformation of initial reactants into products. On the molecular level the mechanism includes, in principle, knowledge of the geometry and relative energy of all structures involved, including isolable or potentially isolable intermediates and transition states, the latter representing the turning points along the minimal energy paths connecting all interconverting species. Following another line of thinking, the reaction mechanism traces the evolution of a chemical system along the reaction trajectory, i.e. the line linking reactant and product molecules in the space of all nuclear coordinates. The concept of a potential energy surface (PES), with all its attendant limitations, is essential to this definition.

MINIMAL ACTION, LEAST MOTION

From such a starting point, the drawing of an analogy with the mechanical description of moving particles is obvious. A predictable consequence was the early application of the principles and methods developed so successfully in classical mechanics to the treatment of mechanisms of chemical reactions. Before the idea of a molecule ever took hold, there had been developed the *principle of minimal action*, first introduced by Pierre Louis Moreau de Maupertuis and universally applied by Leonhard Euler in ballistics, central force motion, etc. According to this principle, spontaneous movements are always associated with minimal changes in the quantity of "action", the latter a well-defined physical variable. Reporting in 1744 to the Académy des Sciences of Paris on the principle of minimal action, de Maupertius stressed, in particular, that light chooses neither the shortest line, nor does it follow the fastest path. Instead, light takes the path which gives real *economy* (cf. the law of parsimony), i.e. where the quantity of action is minimal.[13] Minimal action is itself a beautiful, economic way to get at the heart of physical motion. And it found a place in the new quantum mechanics.

It is thus hardly surprising that when in the 1930's studies of mechanisms of chemical reactions had grown in importance, indeed to become the intellectual focus of the rapidly developing area of physical organic chemistry, the key generalizations relevant to reaction mechanisms were made in the spirit and in the terminology of mechanics. Perhaps, the first step in this direction had been taken even earlier, when J.-A. Muller in 1886, i.e. at a time when molecular theory was still young, introduced *the rule of least molecular deformation* in the course of chemical transformation.[14] The idea was appealing, and found its place in a number of textbooks as *the principle of minimal structural change.*[15] In its most general terms it was formulated by F. Rice and E. Teller, who in 1938 proposed *the principle of least motion* (PLM) according to which. "Those elementary reactions will be favored that involve the least change in atomic position and electronic configuration".[16] In the context of the orbital symmetry rules that were to come into organic chemistry 27 years later, the inclusion of electronic configurations in the Rice and Teller formulation is noteworthy.

To apply the PLM to a certain reaction, the constituent atoms of the molecules of reactant and product must be displaced with respect to one another so that their nuclear motions (usually their squares) are minimized. Indeed, a good number of organic reactions of the rearrangement, decomposition, and elimination type have been shown to follow those reaction pathways that do obey the requirements of the PLM. The extreme simplicity of the relevant computational technique and, more importantly, the clarity of the underlying idea, assured broad application of the PLM treatment of reaction mechanisms, particularly where a choice between several conceivable pathways was needed.[17]

It was always perfectly well understood that PLM represents a very, very simplified theoretical model of the actual motion of nuclei and electrons in the course of chemical reaction. That motion is properly described by the equations of quantum mechanics. None doubted that quantization of electronic, vibrational and rotational states mattered. And that one has to take a dynamic view, describing the real reaction by the totality of the myriad trajectories followed by an ensemble of real molecules in phase space. Still, PLM met a desire for simplicity. Given that it was simplistic, deviations from, or even incompatibility with, the PLM predictions, met in a number of applications of the principle, were never regarded, we think, as final indictments of the inadequacy of a mechanistic hypothesis.

A PERSONAL EXPERIENCE

In contrast to this forgiving attitude toward deviations of a simple theory, the chemical community turns out to be not so tolerant when important, accepted ideas seem to be threatened. Let us give an example, drawing on personal experience.

In 1982 one of the authors (V.I.M.) published a preliminary account of the experimental observation of inversion of stereochemical configuration at a tetrahedral boron center.[18] Several possible reaction pathways that might, in principle, connect the interconverting steroisomers were enumerated. These included (Figure 1): (a) intramolecular (dissociative) and (b) intermolecular (associative) routes, both involving bond-breaking processes at the tetrahedral boron, as well as (c) intramolecular inversion occurring through an intermediate tetracoordinate planar boron species, in which all four bonds to boron are retained (although their strength changes drastically).

Whereas the intermolecular variant of the bond-breaking mechanism was ruled out on the strength of the experimental evidence then available, no unequivocal choice could be made at the time between the two remaining possibilities, (a) and (c).

The Rostov-on-Don authors could not abstain from the temptation of giving preference to the more exciting non-bond-breaking alternative mechanism (c). This choice turned out to be in error, as detailed experimental study later revealed.[19]

But even before convincing evidence in favor of a bond-breaking mechanism was presented, the uncommon interpretation of the "square-planar boron" mechanism of inversion elicited a quick response. Researchers from the University of East

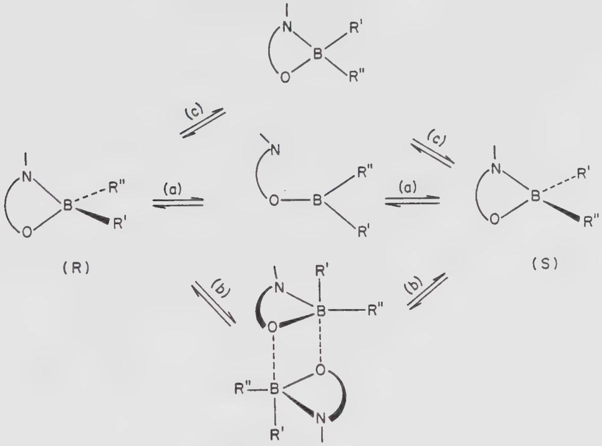

Figure 1

Anglia[20] pointed to the fact that the rate of the inversion process was comparable to that of bond-breaking processes in compounds structurally similar to those studied by the Rostov-on-Don group. On this basis they concluded that the inversion reaction follows the dissociative bond-breaking route, a mechanism with a venerable history going all the way back to the classic 1912 work by Alfred Werner on stereoisomerization of cobalt complexes.

While this was indeed a weighty argument in favor of the bond-breaking pathway, the reasoning of the English researchers was by and of itself not yet conclusive. Perhaps this was why they in turn were seduced by a crumb of philosophy, supporting their argument by the statement that following the dissociative pathway in preference to the bond-conserving inversion "is also a natural result of the application of Occam's chemical razor principle: mechanisms should not needlessly be multiplied."

OCKHAM'S RAZOR AND REACTION MECHANISMS

East Anglia and Rostov-on-Don are hardly enemies; the chemistry got sorted out in the end. Nevertheless, it is interesting to reflect on why appeal to such a general modality of reasoning as OR seemed to be quite appropriate in tackling such a specific problem as the mechanism of a certain chemical reaction? The answer is to be found, we think, in the nature of the theoretical construction which the reaction mechanism represents.

In general, the mechanism of a reaction can neither be directly observed, nor can it be deduced with absolute certainty on purely experimental grounds. It would be nice if the world were that simple. But it isn't. We are not convinced either that femtosecond spectroscopy, an incredibly fast and beautiful way of observing nature, will give the requisite mechanistic answers. The mechanism of a reaction is a logical construction based on a perforce limited set of experimental facts, which are then interpreted by human beings in the framework of current, fashionable and ephemeral theoretical models. And it is logic, with its laws and rules, that makes it possible to arrange observations in harmony with relevant concepts and hypotheses. Ockham's Razor belongs to the category of logical rules which indicate how to process experimental facts. It shows the way to the best fit of observables to the least complicated possible interpretation.

We will return later to some of the hazards of such an "OR-driven" program. But in the present context it is clear that to formulate the mechanism of a chemical reaction is not as simple as it seems. It requires that one not only carry out pertinent experimental (and/or computational) studies, but also that one finds the *most logical explanation* for the findings in terms of existing concepts. It is, therefore, by no means accidental that in many textbooks concerned with the problem of reaction mechanisms, from introductory to advanced ones,[21,22] OR is mentioned among the significant criteria to be met when determining a mechanism. "Mechanisms should not needlessly be multiplied" means that in case several hypotheses match the facts, the simplest one is to be given preference.

Should a chemist regard the chemical and mechanistic version of Ockham's Razor as a universal rule? Could it be violated? The utility of OR in the selection and classification of reaction mechanisms has proven itself in chemistry, just as it has in various other areas of natural science and philosophy.[23] OR must indubitably be counted among the tried and useful principles of thinking about the facts of this beautiful and terrible world and their underlying causative links. But does that make it a rule that should be as inviolable as the First Law of Thermodynamics? We will present arguments that are intended to address this question, as well as the more general issue of the role for OR in the interpretation of scientific data. We will focus special attention on the application of OR in the description of reaction mechanisms. There is epistemological intent in this discussion. But we choose to wind our way through a dialogue of opposing views on how OR has been and should be used, and what the implications of its use may be.

TAKE THAT, YOU NAIVE CHEMIST!

In the preceding section we recited the scientist's catechism, of the great importance and utility of OR. It may come as a surprise to our colleagues that not everyone agrees. For instance, in a remarkably perceptive article, N. Oreskes, K. Shrader-Frechette, and K. Belitz[24] write:

> Ockham's razor is perhaps the most widely accepted example of an extraevidential consideration. Many scientists accept and apply the principle in their work, even though it is an entirely metaphysical assumption. There is scant empirical evidence that the world is actually simple or that simple accounts are more likely than complex

> ones to be true. Our commitment to simplicity is largely an inheritance of 17th-century theology.

Now that puts us right into our place, in the company of ancient priests!

Though, this quote cuts to the heart of the problem, we'd prefer to approach the difficulties with OR gently, through several chemical examples.

MULTIPLE REACTION PATHS

Continuation of the story of the mechanism of inversion of configuration at tetrahedral boron provides the first example. When, in due time, a sufficient body of experimental and computational data had been accumulated concerning the intrinsic mechanisms governing inversion of configuration at a variety of tetrahedral main group metal centers,[25] unequivocal evidence was presented for the simultaneous operation of at least three of the forementioned mechanisms, including the one rejected ostensibly on the basis of OR. Each mechanism has precisely the same net outcome, namely inversion of stereochemistry at the main group metal center. The relative contribution (or energetic preference) of a given mechanism depends on the metal. Structural factors influence the mechanism as well, and may be deliberately manipulated. In some cases (e.g. complexes of zinc and cadmium) all three mechanisms are virtually equivalent in their energetic demands.

Such a diversity of reaction paths for one and the same chemical transformation is by no means a unique occurrence. To nobody's surprise, nature is much more complex than our naive essays at describing it. This complexity becomes so much clearer, the more perfect and sophisticated the methods we employ in reaching for the origins and causes of the transformation of matter that excites us so, and that we call chemistry.

With rapidly developing experimental and computational techniques for studying reaction mechanisms, a good number of important chemical reactions have been found to follow several competing reaction channels, their relative significance sometimes critically dependent on most subtle variation of structure and reaction conditions. This relatively new development may be illustrated by just a few examples.

In the last few years deeper insight has been gained into the detailed mechanism of one of the most important classes of organic reactions, pericyclic reactions.[26] Whereas concerted, i.e. kinetically one-step, pathways represent the principal mechanism, in many cases a biradical-like intermediate (a stepwise mechanism) or transition state becomes competitive, sometimes even preferred. A well-studied example (see Figure 2) is the Cope rearrangement (3,3-sigmatropic shift). Here, even rather tiny structural tuning of the parent hydrocarbon, 1,5-hexadiene, appears to lead to a switch from the most typical pathway (a) with its "aromatic" transition state structure (in two isomeric forms), to pathways (b) or (c), which feature, respectively, a biradical-like transition state or an intermediate.[27]

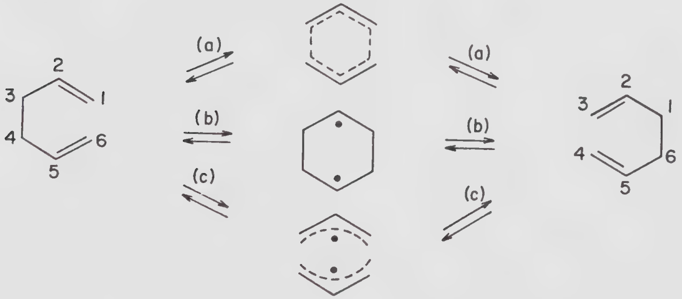

Figure 2

The greater the insight gained into the origin of chemical transformation, the more justified seems the view that reaction pathways are inherently manifold. As we said, one usually thinks of a chemical reaction as a geometric rearrangement of the relative positions of the nuclei which make up the interacting molecules, i.e. motion along a path on the potential energy surface (PES), bisected by ridges that form the reaction barriers. Such a picture of a PES reminds one of a hilly landscape; the metaphor continues with the successfully transformed molecule likened to the motion of a mountaineer moving from the valley of reactants to that of products by surmounting one of the lowest possible passes.

But the real hilly landscapes of this world (or those calculated) are not so monotonous as to feature a unique pass between valleys. Thus branching of reactive trajectories might be a rather common occurrence. The number of trajectories grows rapidly when reactants are supplied with an additional increment of kinetic energy. The requirement of passing through a single saddle point is then relaxed. Moreover, when the nuclear displacements in the course of rearrangement of reactants to products are sufficiently small, the reaction may proceed by a kind of trickling through (under) the energy barrier, i.e. by quantum mechanical tunnelling.[28]

This trend to branching reaction pathways, which seemingly undermines the OR-like comprehension of reaction mechanisms, becomes even more pronounced when one looks at reactions occurring under what might be called extremal conditions —— proceeding with participation of excited states, by electron transfer, subjected to surface catalysis, etc. For an example, let's look at a challenging current mechanistic problem, that of unraveling the mechanism of formation of fullerenes, the polyhedral products of graphite vaporization at plasma temperatures of over 3000 °C. Contrary to an "entropic" expectation of the existence at these conditions of structurally little-organized forms of matter, specific, highly symmetric polyhedral

C_{2n} molecules, their structure reminiscent of the geodesic domes exploited in architecture by R. Buckminster Fuller, are created in carbon vapor. C_{60}, possessing the truncated icosahedral geometry of a soccer ball, has attracted special attention because of the perfection of its polyhedral structure and the horizons opened up with the discovery of a new allotrope of carbon.

How does this thermodynamically unstable molecular soccer ball assemble? Were we to really understand this process, the road to nanometer-scale technology might be open. So considerable effort has been expended on detailed study of the mechanistic aspects of fullerene formation following graphite vaporization.[29] Whereas several ingenious suggestions for the growth process that generates the C_{60} have been forwarded (of these the so-called "pentagon road" model[30] is to us at the present time the most instructive), no model is really compatible with all the known facts, we think. A tiny deviation from optimal reaction conditions found in the famous pulse laser vaporization experiment of Smalley, Curl, Kroto and coworkers appears to result in a drastic decrease of the yield of C_{60}, and in alteration of the mechanism of self-assembly of carbon atoms as well. Noteworthy is the remark made by R. Smalley, one of the discoverers of fullerenes and the advocate of the pentagon road mechanism: "Of course, there must be hundreds of mechanisms whereby a fullerene like C_{60} can form."[30]

Smalley's statement, with which we agree, by no means signifies a repudiation of attempts to gain insight into the detailed mechanism and the driving forces of the spontaneous self-assembly of carbon atoms. The statement merely emphasizes the great complexity of the problem, and the terrible incompleteness of our knowledge.

Let us continue our fault-finding with Ockham's Razor.

ORNATE HYPOTHESES MAY BE RICHER

Supposing there are two explanations for a phenomenon or an observable. Let's symbolize one as

$$\Pi = A \tag{1}$$

where A is the determining factor. The other explanation can be written symbolically as

$$\Pi = c_aA + c_bB, \tag{2}$$

i.e. Π is viewed as being caused by two factors, A and B, in some admixture.

Now it may be that for a single observable Π the "simple" explanation (1) made good enough sense of the available data, and by OR would be preferred to (2). But the universe is likely to have in it not one phenomenon or observable Π, but several, Π_1, Π_2, Π_3... Adducing the more complex explanation (2), even when only one of these phenomena is known, may lead to the eventual realization that there is some related one, Π_2. The more complex explanation is productive, it leads one to think about alternative experiments.

Such an approach may be thought of as one formalization of the epistemologic method of multiple hypotheses that had been advanced at the beginning of this century by Chicago's geologist T.C. Chamberlain and later used by J. Platt (a one-time physicist and chemist) as the basis for the "method of rigorous conclusions".[31] These methods, in a way ramifications of F. Bacon's seminal method of induction, point to the fact that to achieve the right conclusion, simultaneous testing is needed of several hypotheses, each endowed with its own means of uncovering the truth. The summary result of the application of various means and approaches must be richer (and more complete) than the relentless pursuit of a any single hypothesis. Do we need to rehearse the myriad examples the history of chemistry (or our colleagues) provides of the sterility of hypotheses held too strongly, too singlemindedly, by individuals?

COMPLEX NATURE, SIMPLE MINDS

Time and time again the process of discovery in science reveals that what was thought simple is really wondrously complicated. If one can make any generalization about the human mind, it is that it craves simple answers. This is true in politics as in science. So we have a President of the USA (pick any recent one) saying that if we control the flow of drugs across our borders, then we will solve the terrible social problem of drug addicition. Or, just to take something from across the political spectrum, someone (not any President) asserting that if we distribute condoms in the schools that such action will stop the spread of AIDS.

The ideology of the simple reigns in science as well, whereas every real fact argues to the contrary. So we have the romantic dreams of theoreticians (e.g. Dirac) preferring simple and/or beautiful equations. The intricacy of any biological or chemical process elucidated in detail points clearly in the opposite direction.

Let us be specific here, with a chemical and biological vignette, the story of the sex pheromone of the cabbage leaf looper moth, Trichoplusia ni. When the pheromone was first discovered in 1966, it was thought to be a simple molecule, (Z)-7-dodecenyl acetate. A few years later a second active ingredient was found, and more recently some clever biosynthetic reasoning by Biostad, Linn, Du and Roelofs led to the discovery that a blend of six molecules was needed for full biological activity.[32] There is a relationship between the concoction of a new perfume and insect chemistry.

It's not that every physical, chemical, or biological observable needs to have a complicated cause. But we would argue that in the complex dance of ingenuity that is modern science, in the gaining of reliable knowledge, one should beware of the inherent weaknesses of the beautiful human mind. The most prominent shortcoming is not weak logic, but prejudice, preferring simple solutions. Uncritical application of OR plays to that weakness. What's worse it dresses up that weakness in the pretense of logical erudition.

COMPLEX MODELS, SIMPLE MODULES

In our guise as critics of OR, we are, perhaps, guilty of pulling off a philosophical sleight of hand. We (and other critics) imply a necessary relationship between the preference for a simple model and the belief in a simple universe. We then go on to show that the universe is not simple, and thereby appear to invalidate the application of OR in scientific investigation. But does it really follow that one must believe in a simple universe in order to be philosophically honest when invoking OR? Is it not inherent in any analytical epistemology, that one attempt to find simple intellectual bricks from which the wonderfully complex architecture of Nature could be reconstructed? And isn't it really the case that OR properly applies to the identification of these individual modules, rather than to the entire *Weltanschauung* that one builds from them? OR is not a metaphysical statement about the way the universe is; it is a prescription for unraveling and comprehending its marvelous complexity. In this pragmatic point of view, OR serves as an operational principle, not a rule or a Law of Nature.

In the so-called "scientific method," we seek to devise experimental tests that can falsify our hypotheses. The excommunication of ideas that takes place when a model "fails" one of these trials is taken to be rigorous and irreversible, provided that the experimental tests meet criteria of both intellectual validity and competence of execution, therefore reproducibility.

In the pragmatic interpretation of OR, one would not use such irrevocable language. One might say that the choice between two otherwise equally valid models should be made in favor of the simpler, but that the rejection of the more complex is only conditional. The idea that has been set aside could be reconsidered at a later date if the currently favored hypothesis fails some future test. If one adopts such a view, it follows that the temporarily discarded model should not be said to be "ruled out" by OR or to have "violated" OR, since this language belongs in the domain of the more rigorous exclusionary tests.

But even this liberal prescription for the use of OR begs the underlying question of "why?" Why should we lean in favor of the simpler of two otherwise equally satisfactory models? We can advance several arguments, no one of which has logical rigor beyond an appeal to reasonableness.

1. The simpler model is likely to be more vulnerable to future falsification, because with fewer adjustable parameters it will have less flexibility. If, as Popper suggests, a good scientific hypothesis is one that is falsifiable, then perhaps the better of two competing models is the one that is somehow more falsifiable. To be vulnerable is not a weakness, in science or human relationships.

2. Or one could say that the simpler model provides a clearer and more readily comprehensible description. This view would admit the human difficulty with handling complexity, and relate simplicity to comprehensibility. It is important to understand, and the breaking of a complex reality into comprehensible bits is not only the Cartesian method, but a teaching strategy.

3. A third rationale relies on an assessment of the probability of future success of any model. Suppose, in some experiment, we made a series of measurements of a property **y** in its response to adjustment of a factor **x**, with results depicted in Figure 3.

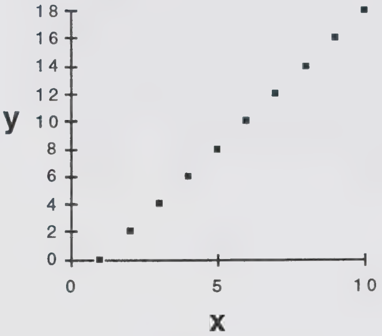

Figure 3

If one wanted to try to describe **y** as some mathematical function of **x**, one would probably choose a straight-line relationship (Figure 4):

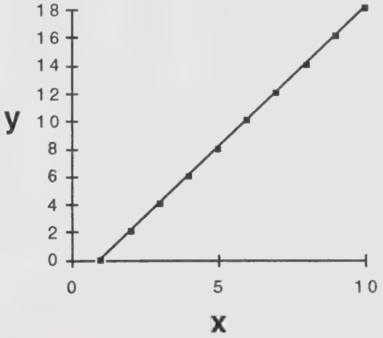

Figure 4

in preference to a more complex functional form such as Figure 5 below:

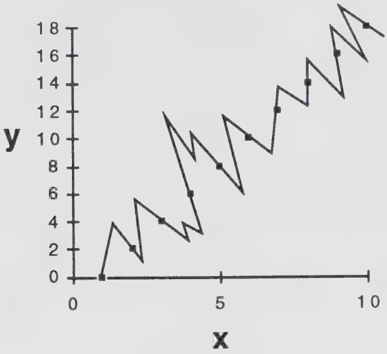

Figure 5

But, aside from some intuitive sense that it just seems right, why would one prefer the straight-line model? An answer can come from looking at the degrees of freedom of the fits. In statistics, the number of degrees of freedom of a model is the difference between the number of independent experimental observations and the number of adjustable parameters in the mathematical function that seeks to describe the relationship between **y** and **x**. It is axiomatic that any function with a number of adjustable parameters equal to or greater than the number of observations can be made to pass exactly through all of the (**x**,**y**) points on the graph. However, it is not necessarily true that a function with fewer adjustable parameters than the number of observations will pass through all of the points. If it turns out that it does, then the function —— our model —— has already had some success in describing one or more events that we have measured experimentally.

The number of degrees of freedom of a model can be thought of as the number of points whose positions were correctly described by the model, without any algebraic requirement that it come out that way. The world is not static. One measurement will be, must be, followed by another. Models that predict are valued. Since we are presumably seeking a mathematical relationship between **y** and **x** in order to predict future points on the graph, we are naturally more inclined to choose the model that has already had the greater success in "predicting" the measurements we have made so far. This will be the model with the larger number of dgrees of freedom, or the smaller number of adjustable parameters —— i.e. the simpler model.

The choice becomes a little less clear-cut when one starts to inquire about models for which the line comes close to, but does not pass exactly through all of the points. In statistical practice, this situation is dealt with by applying the Fisher *F* test.[33] The sum of the squares of the deviations $\Sigma(\mathbf{y}-\hat{\mathbf{y}})^2$ is computed for each model (**y** is the experimentally measured response of the system under study to a given value of **x**; $\hat{\mathbf{y}}$ is the response predicted by the model) and then divided by the appropriate number of degrees of freedom. This calculation provides the variance for each model. The ratio of the variances is compared with tabulated values that allow one to decide, with a specified level of confidence, whether the more complex model has made a statistically significant improvement to the fit. If it has not, one will generally opt for the simpler model because, again, it has the larger number of degrees of freedom.

4. The graphical representation of the **y** *vs.* **x** relationship serves to illustrate a fourth, and here the last, reason for applying OR as an operational principle. The number of equally satisfactory models in a given class is generally related to the complexity of the class. For example, there is one and only one straight line that will pass through all of the (**x**, **y**) points in the graph described above. We do not have to ask which straight line to choose in order to best represent the **x**, **y** relationship. On the other hand, since the number of parameters required to describe the jagged line in the illustration of our more complex model exceeds the

number of observations, there exists an infinity of jagged lines, all passing exactly through the points. With the observations made so far, we have no logically defensible way to choose one from this infinity.

To put it another way, if you think OR gets you into trouble by limiting the number of hypotheses, thereby diminishing the imaginative world, then relaxing from OR opens up real, indeterministic, chaos —— the infinity of hypotheses that fit.

Those of us who have mystically inclined, nonscientist friends may have used arguments like this last one in our discussions of the lack of general scientific acceptance for extra-sensory perception, UFOs, homeopathic medicine, or astrology. The nonscientist might ask: "Do you scientists think you understand everything about how the universe works?" When we modestly profess our woeful lack of understanding, we might hear in return: "Well then how can you rule out the possibility of ...?"

Of course the answer is that we cannot, but in order to make any kind of sense of the world, we must have some procedure for selecting among the plethora of ideas that the collective action of creative human minds has spawned. If we had to operate under an equal opportunity clause for every concept that was ever espoused, we would have such an impossibly complex and self-contradictory description of Nature, that we could never feel that we were making progress in understanding or utilizing our environment.

Why should we make progress? Have we progressed? We are painfully aware of all the ambiguities of the 19th century idea of Progress, in which science flourished. And of the deep mistrust of such progress by thoughtful people in our time. While we're actually ready to do battle for progress, not without internal doubts, this is not the place for that confrontation.

A STATISTICAL INTERLUDE: PRINCIPAL COMPONENT AND BAYESIAN ANALYSIS

The need to have operating principles just to make progress at all in sifting through the complexity of Nature shows up most clearly in the procedure called Principal Component Analysis (PCA).[34,35,36] Many of the observables of nature are multivariate, i.e. each property or phenomenon analyzed yields a series of numbers. Examples are spectra or chromatograms, yielding a datum for each wavelength or retention time. PCA allows one to correlate the data available by deriving a set of orthogonal basis vectors, PCs, so that the first PC represents the best linear relationship, the one showing the greatest variation, exhibited by the data. Each successive PC explains the maximum variance not accounted for by the previous ones. Identifying the number of significant PCs enables one to determine the number of real sources of variation within the data. The most important applications of PCA are those related to; (a) classification of objects into groups by quantifying their similarity on the basis of the PC scores; (b) interpretation of observables in terms of PCs or their combination; (c) prediction of properties for unknown samples. These are exactly the objectives pursued by any logical analysis, and the PCs may be thought of as the true independent variables or distinct hypotheses.

One example of the application of PCA in structural chemistry may be found in the recent statistical analysis of the concept of aromaticity by A.R. Katritzky *et al.*[37] Widely applied for the characterization of specific features of conjugated cyclic molecular systems, the notion of aromaticity lacks a secure physical basis. Not that this has stopped aromaticity from being a wonderful source of creative activity in chemistry. We can think of no other concept that has led to so much exciting chemistry! Yet, although numerous indices of aromaticity have been designed, based on energetic, geometrical and magnetic criteria, no single property exists whose measurement could be taken as a direct, unequivocal measure of aromaticity.

The PCA analysis of the interrelationship of 12 proposed indices for 9 representative compounds indicated that there exist at least two distinct types of aromaticity. "Classical aromaticity" is well described by certain interrelated structural and energetic indices, whereas the second type of aromaticity, the so-called "magnetic aromaticity", is best measured as anisotropies in the molar magnetic susceptibility. It follows from the mathematical treatment that the concept of aromaticity should be analyzed in terms of ornate hypotheses, a multiplicity of measures. But notice that the ornate description is reducible to simple components. The universe is not simple, but the models used to describe it can be made of simple pieces.

Several further examples of the power of intelligent PCA may be found in the recent literature. So Murray-Rust and Motherwell[38] have looked at the molecular deformations of 99 β–1'-aminofuranosides, and have shown a very pretty strong correlation with two PCs, just those expected to define the pseudorotation of the five-membered sugar ring. An analysis of distortions in five-coordinate complexes by Auf der Heyde and Bürgi[39] showed beautifully the relationship of various modes such as the Berry pseudorotation, an S_N2-type mode and an addition/elimination path. And Basu, Gō and coworkers[40] use a PC analysis of molecular dynamics simulations to trace the path of a $3_{10}/\alpha$–helix transformation in an oligopeptide.

There is apparently no obvious equivalence between a PC (or, in general, any other descriptor used in various forms of statistical analysis) and a "physically meaningful" factor which, coupled with strong logic, could provide what we usually mean by "an explanation". The task of combining two or more PC's to provide such factors, along with the search for mutually independent descriptors, is of primary importance in attaining a satisfactory and satisfying connection between logic and statistical models.

Nothing special about chemistry here —— the complexity of this task is illustrated just as well by the difficulties arising in the quantitative description of the perception of quality in food. While from the deterministic standpoint, the quality of a steak or a Bordeaux may be decomposed into attributes or components, sensory analysis demands generation of certain words (factors) used by people to characterize foods.[41]

The science of statistics incorporates OR in its framework in a number of explicit and implicit ways. A particularly useful methodology for fitting models to data and assigning preferences to alternative models is Bayesian inference, introduced by Harold Jeffreys.[42,43] We reproduce here a figure (Figure 6) with its caption from an important article on Bayesian interpolation by D.J.C. MacKay,[44] which succinctly indicates how OR enters the choice of models in this methodology.

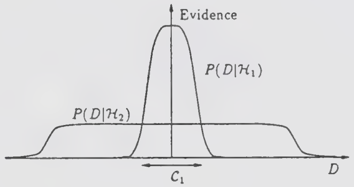

Figure 2: Why Bayes embodies Occam's razor. This figure gives the basic intuition for why complex models are penalized. The horizontal axis represents the space of possible data sets D. Bayes rule rewards models in proportion to how much they *predicted* the data that occurred. These predictions are quantified by a normalized probability distribution on D. In this paper, this probability of the data given model $\mathcal{H}_i$, $P(D \mid \mathcal{H}_i)$, is called the evidence for $\mathcal{H}_i$. A simple model $\mathcal{H}_1$ makes only a limited range of predictions, shown by $P(D \mid \mathcal{H}_1)$; a more powerful model $\mathcal{H}_2$, that has, for example, more free parameters than $\mathcal{H}_1$, is able to predict a greater variety of data sets. This means however that $\mathcal{H}_2$ does not predict the data sets in region C_1 as strongly as $\mathcal{H}_1$. Assume that equal prior probabilities have been assigned to the two models. Then if the data set falls in region C_1, the *less powerful* model $\mathcal{H}_1$ will be the *more probable* model.

Figure 6

We return to our dialogue, to question the arguments made in favor of an operational valuation of OR.

WORLD VIEW OR OPERATING MANUAL?

If we distance ourselves from philosophical implications by treating OR as just an operating principle, aren't we really displaying intellectual cowardice? Take that straight-line graph. If we made the measurements leading to the (**x**, **y**) points already shown, wouldn't we really believe that the "proper" value of **y** at some new value of **x** within the range would be the one that fit on our straight line. Indeed, if we didn't obtain such a result wouldn't we suspect that we had made a mistake in our experiment? And isn't such an expectation really a belief in a simple universe?

In the processing of models we must be especially cautious of the human weakness to think that models can be verified or validated.[24] Especially one's own. The main tactical problem in modeling the course of chemical reactions, be they ozone depletion or a pericyclic reaction under new conditions, is to find a reasonable balance between completeness of description of an object or phenomenon under study, and the simplicity of the models applied. The balance is really, really delicate and the razor (OR!) is best wielded by a really skillful barber (experienced chemist) to warrant that essential but hidden features of the object under study were not lost upon modeling its properties and behavior. In the United States, at least, there are not too many barbers left who can give you a razor shave.

SMOOTHNESS AND SIMPLICITY

The dialogue is not finished. When one infers a linear relationship from empirical observation, be it a linear free energy relationship in physical organic chemistry, or a Hooke's-Law relationship in physics, one would indeed be surprised if some of the measurements, made within the range of all the others, failed to fit the model. But that surprise derives not from belief in a simple universe, but rather from belief in a smoothly changing one. With the important and fascinating exception of systems on the threshold of chaotic behavior, our experience suggests to us that the universe is much more a system of smooth curves than jagged edges. It is not often that small changes in some control factor cause wild and unpredictable swings in the response of the system under study. We understand now the importance of bifurcation points in chaotic systems, and know that complex assemblies are subject to chaotic behavior.[45] But most of chemistry is a science of smooth trends. While nobody believes that the plot of free energy of activation *vs.* standard free energy of reaction is well described by a straight line for all reactions, we can restrict our attention to small enough changes in the structures of the substrates so that the smooth relationship between activation and reaction free energies can reasonably well be approximated by a straight line.

The observations of the "facts" about the universe that can appear to make it complex, multichanneled, and poorly described by smooth models are actually not really as objective and independent of our conceptual prejudices as we might like to think. Take that Cope rearrangement again. For a while it looked like the compromise between the "aromatic" and "biradical" camps was to say that both were right, and that the system flipped from one mechanism to another in response to changes in substituent, as we have described. Such a flip-flop would not be easily described by any linear or smoothly curved function. However, the latest, highest-level *ab initio* calculations have returned us to a smoother description.[46] The multiplicity of reaction channels has disappeared again, and we are now in a situation where the best model seems to be one in which the geometry of the transition structure moves smoothly and continuously from "aromatic" to "biradical" in response to substituent changes.

Even the duality of "concerted" *vs* "stepwise" mechanisms may be falling to a smoother description. The forced choice between such descriptions is, at least in some cases, a consequence of drawing a potential energy profile in which there is only a single dimension assigned to the reaction coordinate. One then has only two options: one includes a little dip in the curve to imply the existence of an intermediate along the reaction coordinate (stepwise), or one does not (concerted). But of course, for a nonlinear, N-atom molecule there are 3N-6 dimensions to the reaction coordinate. In this space, there is no need to place a local minimum in the potential energy surface on an obligatory path between reactant and product. If such a local minimum exists, and if it is energetically accessible without intervening barriers, then should it be called an intermediate or not? Is the reaction concerted or stepwise? The two descriptions merge smoothly together.[47]

Some barbers will use OR to give you a smooth shave.

MODELS, PARADIGMS AND REVOLUTIONS

Continuing our arguments for...

The gap between the complexity of an object under study and comprehension of its origin is bridged (shaky constructions, to be sure...) through elaboration of suitable models devised to describe the underlying features of the object under study in terms of previously understood phenomena. Every model is, by definition, incomplete.[48] It is thus hardly surprising that a set of complementary models, each of them valid over a certain range of application, is generally needed to describe adequately an object as a whole.

We would like to forward a tentative notion that in the evaluation of models, different criteria may be applied whether one seeks understanding or predictability. We enter an epistemological battleground here (deep trenches recently dug on the field of artificial intelligence...) in positing that there is difference between human understanding, perforce qualitative, and that dream of dreams, a computational model that predicts everything accurately.[49]

Real chemical systems, be they the body, the atmosphere, or a reaction flask, are complicated. There will be alternative models for these, of varying complexity. We suggest that if understanding is sought, simpler models, not necessarily the best in predicting all observables in detail, will have value. Such models may highlight the important causes and channels. If predictability is sought at all cost —— and realities of the marketplace and judgments of the future of humanity may demand this —— then simplicity may be irrelevant. And impossible, for, as we said, any real problem is complex and will force a complex model. Whatever number of equations or parameters it takes, that's fine. As long as it works.

Ockham's Razor is a conservative tool. It cuts out crazy, complicated constructions and assures that hypotheses be grounded in the science of the day. So the tool is certain to lead to "normal" science, the paradigmatic explanation. Revolutions in science, to follow Thomas Kuhn's fruitful construction, do not grow from such soil.

Perhaps that is an oversimplification. At the critical turning point when a revolution is about to break loose, OR can turn a conservative into a reluctant revolutionary. We're thinking of Max Planck, interpolating between the Wien and Jeans radiation laws, and following the logic, an OR logic, to the quantum hypothesis. And, it seems, resisting that hypothesis even as the world and he found it necessary.[50]

And against...

TELLING STORIES, TELLING IT STRAIGHT, WRITING POETRY

There was spoken language before writing, before science. And around the fire, when men and women sat and talked of the things of this world, even then there were different ways of telling the story of a failed hunt, of an insect from which one could make a red dye, or what needed to be done to a certain rock to win from it a hard metal. The stories could be embroidered, and gods pulled in as causes. No one suffered from these tales, in fact they provided a spiritual matrix for the material world.

Then there came science, and the ritual way of reporting it, the scientific article. To gain reliable, repeatable knowledge, to deal out of the game prejudiced natural philosophers, the narrative in the standard article tightened. But if you think that scientific articles tell the facts and nothing but the facts, please look again. The facts by themselves are indigestible. They are, and must be, encased in language, connected to frameworks of understanding (theories). Try writing an article with just the facts, and see how many people read it! The narrative may be suppressed (which actually, as suppression usually does, only raises the tension lurking beneath the surface) but the impulse to tell a story remains.

With no nostalgia for those days around the fire, the wielding of Ockham's Razor attacks something most fundamentally human, the love for narrative. There are times when the story has to be told simply, the fire engine sent the shortest route to the fire. But a world without stories is inhuman. It is a world where nothing is imagined. Could a chemist be creative in such a world?

Let us put it another way. There is a human tendency to tell elaborate stories if not tall tales. Even scientists succumb to it. And there is a logical emphasis on the succinct, the unembellished, which has certainly been part of the successful method of science. There is danger in going astray, following the person who tells a wild story well. And there is danger —— we think perhaps greater —— in telling too few stories, in building fewer scenarios which present or future facts may demolish. Or uphold.

There is another very human literary activity. This is to write poetry, to tell essences intently, in words. Curiously, the cult of beauty as mathematical simplicity represents a reaching for essences that parallels the compact truth-telling that is poetry. This is what Dalton, Dirac, and Einstein aspired to. But poetry is more. Not a stripping to a common nakedness, it aspires to singularly adorned simplicity.

OCKHAM'S RAZOR AND THE STRUGGLE FOR UNDERSTANDING

The search for true understanding might be compared with the crafting of an endless, absorbing mosaic picture. The pieces already in place, lustrous and dull, have been laboriously and joyously shaped in the creative work of thousands of years of protoscience and a few hundred of "real" Western science. They furnish us with some clues as to the nature of the beast. If simplicity of interpretation (in other words, "beauty of equations," according to P.A.M. Dirac, or "lucidity complementary to truth," according to N. Bohr) be a desirable quality, the interpretation must be constructed out of simple[51] components. The principle of parsimony is then just what we need as we labor, discover, and create.

If the desideratum be a human science open to change and the unexpected, then maybe there are occasions when OR should be sheathed. Or we should remind ourselves ceaselessly of the conditional interpretation of a conclusion based on OR reasoning. Cognizance of the complexity that so beautifully contends with simplicity in this evolving world, cognizance of the creative foment of intuition without proof within science, lead us to think so.[52]

Intuition figures prominently in the strong pull on us toward the simple, the logical, and the beautiful. Plato had that right. And the same word, intuition, serves us as we argue for a certain sterility of William of Ockham's sharp principle. "Intuitive" is, probably, the best characterization of the law of parsimony, Ockham's Razor. It is precisely human intuition that provided and provides for the disclosure of those mysterious and wondrous ways of Nature, and the creation of so much new. The mosaic grows. And it was also intuition that sometimes led to the oh so many blind alleys, if not mistakes, of our sciences...

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[32] Of course it takes six for sex: Bjostad, L.B., C.E. Linn, J.-W. Du, W.L. Roelofs, "Identification of New Sex Pheromone Components in Trichoplusia ni, Predicted from Biosynthetic Precursors." *J. Chemical Ecology*, **1984**, *10*, 1309-1323. W.L. Roelofs and T. Glover. *Genetics of a Moth Pheromone System*, in *Chemical Senses*, Vol. 3, C.J. Wysocki and M.R. Kare, eds., New York, Marcel Dekker, 1991. C. E. Linn and W.L Roelofs. *Pheromone Communication in the Moths and Its Role in the Speciation Process.* to be published.

[33] See, for example, J.C. Miller and J.N. Miller *Statistics for Analytical Chemistry*, 2nd ed., Ellis Horwood, Chichester, **1988**, p.60.

[34] E.R. Malinowski and D.G. Howery, *Factor Analysis in Chemistry*, Wiley-Interscience, New York, **1990**.

[35] See also H.G. Gauch, Jr., *Amer. Sci.*, **1993**, *81*, 468.

[36] T. Auf der Heyde, *S. Afr. Chem. J.*, **1993**, *46*, 45.

[37] A.R. Katritzky, P. Barczynski, G. Musumarra, D. Pisano, and M. Szafran, *J. Am. Chem. Soc.*, **1989**, *111*, 7-15.

[38] P. Murray-Rust and W.D.S. Motherwell, *Acta Crystallogr., Sect. B*, **1978**, *34*, 2534.

[39] T.P.E. Auf der Heyde and H.-B. Bürgi, *Inorg. Chem.*, **1989**, *28*, 3960, 3970, 3982.

(..continued)

[40] G. Basu, A. Kitao, F. Hiratu, and N. Gō, *J. Am. Chem. Soc.*, **1994**, *116*, 6307-15.

[41] See "toughness-tenderness" and "juiciness" separated as important PCs in an analysis of 69 beef roasts by J.M. Harris, D.N. Rhodes, and B.B. Chrystall, *J. Texture Stud.* **1972**, *3*, 101, or the analysis of sensory characteristics of ham and their relationships with composition, visco-elasticity and strength: G.R. Nute, R.C.D. Jones, E. Dransfield, and O.P. Whelehan, *Int. J. Food Sci. Tech.*, **1987**, *22*, 461. Our source for these references on sensory properties and preferences of meat products is a perceptive overview by Einar Risvik, (Matforsk, Ås, Norway), to be published.

For the use of PCA in the evaluation of 1976 Bordeaux wines see A.C. Noble, A.A. Williams, S.P. Langdon, *J. Sci. Food. Agr.*, **1984**, *35*, 88. H.K. Sivertsen and E. Risvik (to be published), have carried out a detailed multivariate study of French wine profiles. They had eight panelists rate thirty wines for 17 specific and integrated sensory attributes. Two PCs accounted for 65% of the variation. The first of these was a fruity aroma axis, "going from berry aromas to vegetative aromas and attributes representing a more ripened aroma, like 'animal' and 'vanilla'. PC2 could be described as a mouthfeel and color axis, going from 'suppleness' to 'astringency', 'color intensity', 'potential,' and 'color tone'." Sivertsen and Risvik point to an amusing mapping of the wine varieties separating along these PCs onto the geography of French wine-producing regions.

[42] H. Jeffreys, *Theory of Probability*, Oxford Univ. Press, Oxford, **1939**.

[43] See also articles by S.F. Gull in *Maximum Entropy and Bayesian Methods in Science and Engineering, Vol. 1. Foundations*, G.J. Erickson and C.R. Smith, eds.,Kluwer, Dordrecht, pp. 53-74, and in *Maximum Entropy and Bayesian Methods, Cambridge 1988*, J. Skilling, ed.,Kluwer, Dordrecht, pp. 53-71.

[44] D.J.C. MacKay, *Neural Comput.*, **1992**, *4*, 415-447.

[45] H.G. Schuster, *Deterministic Chaos*, Verlag Chemie, Weinheim, **1984**.

[46] D.A. Hrovat, K. Morokuma and W.T. Borden, *J. Am. Che. Soc.*, **1994**, *116*, 1072-1076.

[47] B.K. Carpenter Acc. Chem. Res., **1992**, *25*, 520-528.

[48] C.J. Suckling, R.E. Suckling and C.W. Suckling, *Chemistry Through Models. Concepts and Applications of Modelling in Chemical Science, Technology and Industry*, Cambridge University Press, Cambridge, **1980**.

[49] For a contrary view, see: H.A. Simon, *The Sciences of the Artificial*, 2nd ed., MIT Press, Cambridge, **1981**.

[50] M. Jammer, *The Conceptual Development of Quantum Mechanics*, 2nd ed., American Institute of Physics, New York, **1989**.

[51] It is not all that easy to define simplicity "The notion of simplicity, like truth, beauty and effective process is an intuitive one calling for a more objective characterization, i.e. formalization, before we can even hope to agree about the relative complexities of different theories" (J. J. Casti, "Searching for Certainty," *An Abacus*, London, **1993**, 349).

[52] Still another perspective, one which should make a scientist stop and think, comes from a sensitive reader of this paper, sympathetic to science. He

(..continued)

remarked that to most nonscientists, the very idea that OR is part of the scientific method seems strange. This is because to many, science is not about simplicity, but about complexity. Our enterprise seems difficult and obscure to people, even as they use the fruits of that greater knowledge of the world.

THE SAME AND NOT THE SAME

Roald Hoffmann

June 16, 1994

PREFACE

In this book I argue that chemistry is interesting, both to the practitioners of the molecular art, craft, science, and business, and to the reflective consumers of its products. The interest derives from an inherent tension. Each fact or process of the science, and the way these are viewed, is in precarious balance between polar extremes. And the polarities of substances and their transformations resonate with forces deep in our psyche.

1

What do you want when you come to a physician with your aging father, weak and feverish? Compassion to be sure, but also a laboratory workup of blood chemistry, or a test for the organism possibly causing the suspected pneumonia. And, if needed, a drug, an antibiotic tailored to remove that organism from your father's body.

What do I scream about when the town decides to put a huge garbage incinerator, taking in municipal and industrial waste from around the state, next to my home? It's the traffic, the smell, the possible discharges into my well water of certain ions and molecules, still other pollutants into the air.

The substances you desire from the physician, the substances I worry will turn up in my air and water are chemicals. So are you, and I — chemicals, simple and complex. You certainly want more than a prescription of some chemicals from a doctor — you

want care and compassion. And I want more than reassurance and continual monitoring of chemicals emitted from the agency that sites the incinerator — I want fairness, a real consideration of environmental impact, and of alternatives to incineration. But in the material, real world, we, you and I, deal with and react to substances that are chemical.

These chemicals we desire and fear (chemists call them compounds or molecules, once they are reasonably pure) are not the largest (the realm of astronomy), nor the smallest (part of physics). They are squarely, nicely in the middle, on our, human, scale. Which is why we care about them, not as distanced, hypothetical constructs, but in this world. Those molecules, of pharmaceutical or pollutant, are of just the right size to interact, for better or for worse, with the molecules of our bodies.

That a reasonable human being can be ambivalent about chemicals, seeing in them both harm and benefit, is not a sign of irrationality, but of humanity. Utility and danger are two poles of a duality. Any fact in our world is evaluated, often subconsciously, by our wonderfully rational and irrational mind, in terms of such polarities. Only if one is dead to experience does one fail to ask the dual question — "Can it help me?", "Can it hurt me?" Asking that question endows the object of the query, the "it", with a kind of life. It is linked to you. The tension of the object being harmful, or harmless, or maybe both, makes it interesting. The tension of asking the question and struggling

with the answer links the material and spiritual worlds.

Harm or benefit, harm and benefit, is only one of the polarities which makes chemistry interesting. In this book I will explore others as well. The first will be that of identity. As the title of this book implies, I happen to think this is the most important one. Later on, I will look at dualities such as static/dynamic, creation/discovery, natural/unnatural/ and to reveal/to conceal.

A chemical fact — a molecule, a reaction — is poised in some way in the many-dimensional real and mental space defined by these dualities. Is it a new molecule, or one made before? Is it safe, or harmful, and to whom? Is it sitting still, the way it seems to, or is it really moving at the speed of sound? Is it present in nature, or made in the laboratory? Question after question; questions that build tension, especially if the answer is "neither", or "both". Tension gives life, the potential of change. If there is anything central to chemistry, it is change.

2

There is a second, connected aim of this book — to tell you what chemists really do. I don't intend to propagandize for chemistry, but to open to you a window into the chemist's world. So that you may see how these dualities, connecting up with psychological forces common to all us, enter the life of the practitioners of the art.

To understand is to give oneself the possibility of not being afraid, perchance be interested. The chemists' world is

penetrable. Through case studies I will show you how intellect and tools are marshalled to answer the simple questions anyone would ask: "How do I do it?", "What do I have?", "How did that really happen?", "How shall I tell others, if I am to tell them?", "Is it of value?".

Answering these simple common language questions leads one quite naturally to ponder the dualities underneath. So, asking "What do I have?" becomes "Is this white powder the same or different from a million white powders (yes, there are a million, at least) made previously by others?" I will try to show you, by example, how practicing chemists deal with these questions.

3

Since the theme of polarities I stress bridges matter and emotion, there is no way to avoid the human person, with his or her immense capacity for curiosity, bold creation, and fear. I will discuss the thalidomide episode, a failure of the system and of individuals. And I will tell of the complicated creative and tragic life of a great German chemist, Fritz Haber. I will make a personal statement of what I see as the social responsibility of scientists and an equally personal one on how a chemist might respond to environmental concerns. My aim is for a middle ground, as hard as that may be to find.

4

Chemists are no more reflective than other people. But the questions they pose, and the craftsmanship with which they answer them, move them to consider polarities, and the associated

tensions. Or the dualities press themselves, subconsciously, into the chemist's mind.

The dualities, of molecules and the process of their making, are important, I think, in forming a linkage between the chemist and the non-chemist. It is possible to answer the question "What do I have?", and to reflect on whether the substance made is the same or not the same as others. But why is that question interesting? Because the question of identity, of our identity, shaped in childhood in a complex dance of bonding and separation, matters deeply to us. The processes of nature connect up to the interior world of our emotions.

Identity and deception, origins, good and evil, sharing and withholding, overcoming obstacles, resurrection, danger and safety are some of the psychological constructs or mythical structures with which the world of molecules connects. These emotional focal points shape, consciously and subconsciously, the wonderful, game-playing psychology of the chemist engrossed in molecules. It helps to see this to sense what moves chemists. And I think the material-psychological link, expressed through polarities, allows us to understand why we like and fear chemicals.

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LIVES OF THE TWINS

Joyce Carol Oates, one of our most talented and prolific writers, has recently written several psychological thrillers under a poorly concealed pseudonym, that of Rosamond Smith. In one way or another these novels deal with the complexity, richness, and threat of twinhood, with similarity and difference.

In "Lives of the Twins", published in 1987, Oates/Smith draws us into the world of a young woman, Molly Marks, who falls in love with her therapist, Jonathan McEwen. It emerges that Jonathan has an identical twin, James, whose existence he has concealed from Molly. Some hidden dark evil has separated the twins. James is also a psychotherapist. Molly, obsessed, seeks out James and begins a complicated relationship with him. Here is Molly's description of the brothers:

> Yes, their hair whorls in opposite directions but it *is* the same hair, precisely — texture, thickness, springiness, degree of silvery-gray streaks and shadings...If their teeth tend to decay on opposite sides of their mouths Molly can't know but, in all, their teeth look very much alike. Each has a slightly jagged left incisor that gives him, to Molly's romantic eye, a rakish razorish air, like Mack the Knife...When Jonathan smokes he holds his cigarette in his right hand, and, exhaling smoke, has a habit of screwing up the right half of his face; James holds his cigarette in his left hand, and, exhaling a luxurious cloud of smoke, screws up the left side of his face. Jonathan appears to smoke only when he is unhappy while James, who is never, evidently, unhappy, smokes when he pleases. James smokes the brand of cigarettes Jonathan smoked when Molly first knew him; now Jonathan is trying other brands, less potent, and less satisfying, in an effort to stop smoking entirely.
>
> Both brothers use the same brand of razor blades, deodorant, aspirin, toothpaste...though James squeezes

the toothpaste tube anywhere he wishes while Jonathan squeezes it from the end and neatly rolls it.[1]

What do the sometimes identical, sometimes mirroring habits of a set of fictional twins have to do with chemistry?

Chemistry, the molecular way of knowing the natural and unnatural, is a remarkable science, prodigal in the way it has changed our world. Chemistry touches every aspect of the way that we live — James' and Jonathan's razor blades, deodorant, aspirin, toothpaste indeed. We wear clothes in colors that were once accessible but to potentates, we live when we would have died many times over. Illustration 1 shows the rate of survival in children afflicted by a variety of solid tumors, plotted as a function of year in this century. Not much happens until chemotherapy is introduced.

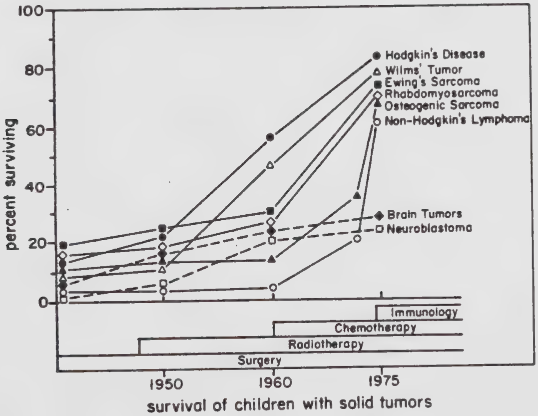

Illustration 1: Percent survival of children diagnosed with various types of solid tumors over the period 1940-1975.

Through the science of molecules and their transformation we have learned of the invisible inside of matter, the prolific ways in which atoms link up in natural silk and artificial nylon. And we wash our apples not so much because of the dirt on them, but because we're afraid of the chemical residues another part of ourselves has put on those apples. Illustration 2 shows a chemical dump site; inefficient industrial production and human failure sometimes combine to pollute our environment.

Illustration 2: A chemical dump site. *(Photo by John Cunningham/Visuals Unlimited).*[2]

All this, in the complex beauty of the real world, totally resistant, as human personality is, as art is, to simplistic categorization as good or evil — all this is chemistry. The

Janus image is a fit summary of how much of the outside world regards chemistry.

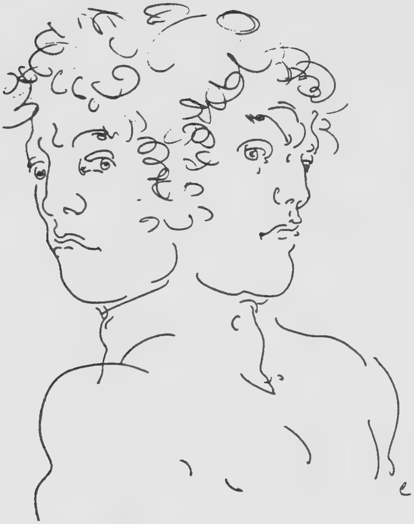

Illustration 3: Janus, by Hans Erni.[3]

The ambiguity in the way chemistry is perceived is but one, external, dichotomy. There is more. Poised centrally between the physical and biological universes, chemistry doesn't deal with the infinitely small or large, nor with life. So it is sometimes typed as dull in the way things in the middle are. But there is a dual surprise awaiting the careful observer of the molecular scene; it's a rich, agitated world down there, both in its innards and in the emotions of the supposedly dispassionate

but impassioned practitioners of molecular arts. In this book the essential tensions of chemistry will be explored; I will seek the polarities that power, rend and reform the world of molecules.

What do twins have to do with it? Everything. The questions implicit in Molly Marks' description of the twins are: "Who are you?", "Are you different?", "Are you the same?" The tension for Molly is that of recognition, of identity, of the same and not the same. The same overpowering questions initiate the dialogue of a chemist with recalcitrant matter. He or she also asks "What are you?", "Are you different?", "Are you the same?" The stranger within; molecular mimicry — these guiding metaphors of immunology and drug design extend the notion of molecular identity. They are strong metaphors, as we will see, because they touch deep concerns, of differentiation, individuation, the self.

1. Rosamond Smith, Lives of the Twins, (New York: Simon and Schuster, 1987), p. 102-3.

2. Reproduced by permission from M.D. Joesten, D.O. Johnston, J.T. Netterville, and J.L. Wood, World of Chemistry, (Philadelphia: Saunders, 1991).

3. From Panta Rhei, Vol I, (Luzern: Hans Erni-Stiftung, 1981), p. 83.

WHAT ARE YOU?

The very first question that a chemist asks when faced with a sample of anything new under the sun — some dust brought back at fantastic expense from the surface of the moon, an impure narcotic off the street, an elixir extracted from a thousand cockroach glands — is the same: "What do I have?" This query turns out be more complicated than one thinks, for in this real world everything is impure. If you were to look at the purest things in our environment — silicon wafers, table sugar, or some pharmaceuticals — you would find that at the parts per million level, you would not <u>want</u> to know what is in there!

Everything is in fact quite dirty. Especially natural things, which are much more impure on the average than synthetics. Nicely so. Some 1200 aroma components have been found in white wine; that great German Mosel, the 1976 Bernkasteler Doktor Trockenbeerenauslese, is identified by the expert taster because of the <u>mix</u> of ingredients, chemicals (what else is there?) which give the wine its taste and smell. Curiously, the taste and smell as a whole, even though the ingredients are chemical and can be quantified, elude the chemist's expertise. It takes a wine person, a palate and a nose, to pick that wine out.

Why are natural things impure? Because living organisms are complex and they are product of evolution. You need thousands of chemical reactions, a myriad of chemicals to "run" a grape, or

your body. And nature is a tinkerer; the solutions for ensuring survival of a plant or animal are the result of millions of years of random experimentation. The patches on the fabric of life come in a bewildering variety of molecular shapes and colors. Anything that works is coopted. And banged into shape by all those natural experiments.[1]

So the realistic question becomes not "What is it?", but "How much is there of what?". One must separate a substance into its constituent components. Each component is a compound, a persistent grouping of atoms that stick together. That group of atoms is called a molecule; a pure compound is a substance consisting of a very large (molecules are tiny) assemblage of identical molecules. Each compound will have quite different properties; sugar and salt may be white crystalline solids soluble in water, but there's no problem in distinguishing them by other physical (and chemical, and biological) attributes.

After separation of a substance into its components, one wants to identify the constituent compounds. To a chemist "structure" means the identity of the atoms that are in the pure compound, how those atoms are connected to each other, and what their arrangement in space is.

Let us begin with the problem of separation. I happen to be a mineral collector; Illustration 4 below shows one way nature does it; cubic crystals of fluorite, clear to pale lavender, perch on long-bladed crystals of barite in this specimen from the Schwarzwald, Germany. If you have time, of a geological scale,

available to you, then, under certain conditions, substances might separate from each other naturally, as these did. The method is called fractional crystallization. Most chemists' patience is not on the order of thousands of years. The five

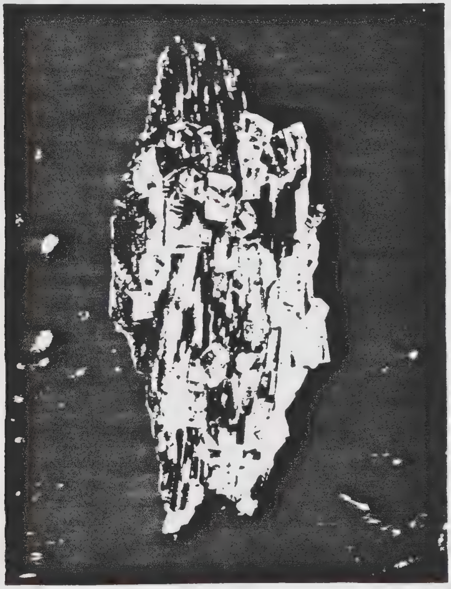

Illustration 4: Fluorite on barite[2]

years that a Ph.D. student spends in graduate school is more like

it. Human beings want a speedier technique, and so one invents machines to separate things.

Illustration 5 is the outcome of such a machine at work. This "gas chromatograph" may cost about 5 kilodollars. It separates molecules by a repeated process of adsorbing them on little sand-like grains, then releasing them. In this duality of holding on and letting go, different molecules find a different balance, and pass through the machine slower or faster.

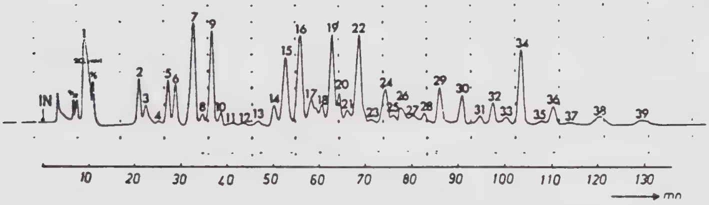

Illustration 5: Thirty nine peaks, each containing at least one compound from the aroma of cocoa. The horizontal axis is time, in minutes, in which the compound is eluted from a gas chromatograph. The vertical axis is related to the concentration of the components.

The article from which this illustration is taken describes the work of a group of chemists engaged in analyzing the aroma of fresh cocoa.[3] Why would anyone want to do that? The Nestlé laboratories in Vevey, Switzerland might well want to do that. Their chemists took a mere 2000 kilograms of Ghanaian cocoa, extracted the aroma with steam and dichloromethane. They concentrated the extract to just 50 milliliters. Then they put

fractions through the gas chromatograph. In the illustration you see 39 peaks on some time scale, emerging from their ordeal of union and separation in the chromatograph. Every one of those peaks is at least one compound; the Nestlé chemists actually identified 57 different compounds, 35 of which had not been previously known to be in cocoa. The complexity of the real world swims out at you. It may not be that all 57 compounds (each made up of a lot of identical molecules) are necessary to give the aroma of cocoa. But it's remarkable how complicated that natural mixture is.

The next task is to find out precisely what molecules are in each one of these 39 peaks. In some cases, when the molecules cooperate, if they crystallize neatly, then, with a machine called an X-ray diffractometer (costing about a hundred kilodollars) and one man- or woman-week of work, it is possible to determine the structure of the molecule.

An example of such a "crystallographically determined" molecular structure is shown in Illustration 6.

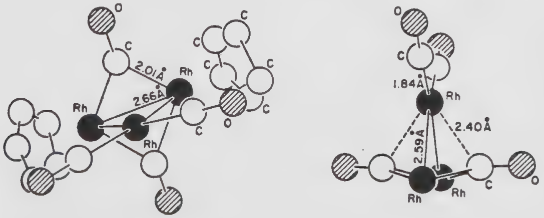

Illustration 6: Two views of the structure (in a crystal) of $Rh_3(C_5H_5)_2(CO)_4^-$.[4]

This is not a molecule to be found in the aroma of cocoa! It has three rhodium atoms in it — as far as I know no one has found precious rhodium in cocoa. Not that natural organisms avoid metals; there is a central role for iron, copper, manganese, zinc, magnesium and even rare molybdenum and selenium in living systems. But rhodium, critical for the operation of your car's catalytic converter, isn't an essential biological trace element. I show the molecule just to indicate the detail in which one can determine molecular shape. In this Star Wars representation you see some numbers; those are distances between the atoms. Even such metrical detail may be gleaned.

1. F. Jacob, "Evolution and Tinkering," Science 196 (1977): 1611.

2. Reproduced by permission from Mineral Digest, 3 (1972): p. 71. Photograph by Studio Hartmann.

3. J.P. Marion, F. Müggler-Chavan, R. Viani, J. Bricout, D. Reymond, and R.H. Egle, "Sur la composition de l'arôme de cacao," Helvetica Chimica Acta 50(6): 1509-16.

4. W.D. Jones, M.A. White and R.G. Bergman, J. Amer. Chem. Soc. 100 (1978): 6770-3.

WHIRLIGIGS

Yet often molecules do not cooperate with us, telling us their mysteries so directly. They may just fail to give the nice little crystals requisite for the technique described at the end of the last section, X-ray crystallography. Let me tell you a little story of how some chemists determined the structure of a molecule when a direct crystallographic solution was not available. The story is drawn from the work of colleagues of mine, Jerry Meinwald, an organic chemist, and Thomas Eisner, a neurobiologist, entomologist, and insect physiologist, both at Cornell. They have been working together for the last 30 years on chemical ecology, the defense and communication systems of insects. Insects are the greatest chemists. More than other spieces they use successfully simple and complex molecules, singly and in perfume-like blends, to communicate in feeding, defense, reproduction and behavior.[1]

You see a typical scene near my home town of Ithaca in Illustration 7. It is autumn, our finest season, maple leaves floating on the surface of a pond. On that surface are some little beetles. These interesting organisms, whirligigs, family Gyrinidae, live in a unique habitat, on the surface of water. The aspiration of many a fisherman is to simulate the scenario of Illustration 7, an insect moving on the surface of the water. Since whirligigs proliferate, Eisner reasoned that they might have a defense mechanism against predating fish and amphibians. He set out to determine that mechanism.

AN ATTRIBUTE OF THE DEVIL

is what Wolfgang Pauli called dichotomizing.[1] It is too easy. And ultimately tiresome. But there is a difference between just listing opposite qualities (good/evil, symmetry/asymmetry) and coming to terms with the tense synthesis of opposites that makes life interesting. So neither men, women nor molecules are exclusively good or evil, and if beauty is to be found it surely is at the edge where symmetry and asymmetry contend.

There is a philosophic perspective that seems on the surface close to the road I've followed in analyzing chemistry — the Hegelian dialectic. Hegel proposed a mode of argumentation that was also a presciption for understanding. For any thesis there is an antithesis. From the contention of the two there evolves a synthesis. (We can't get away from this word!)[2]

A way of polarities or dualities certainly has a dynamic that resembles the working of Hegel's dialectic. But I think our way of looking at chemistry moves beyond dualism, in two ways. First, the chemical fact, or the act of the chemist on obtaining that fact, is a balancing act on the polar axis — a different compromise for every molecule, every maker of that molecule. Second, there is not a single thesis or antithesis, but a multiple perspective, if not cubist at least many-dimensional.[3] A molecule may be similar to another one, harmful or beneficial, discovered or created, quiescent or in rapid motion. Under certain conditions, it may be all of these!

Why opposition? I think there is little choice but to focus on polarities in describing a living, changing <u>human</u> activity such as chemistry. Here is what Emily Grosholz, a poet and philosopher, says in her remarkable essay on nature and culture in two books by W.E.B. Du Bois:

> Metaphysical schemes that accord reality to development must display the structure of reality in terms of possible changes; change requires difference, and difference takes the form of binary oppositions in our language and thought. The venerable binary oppositions of metaphysics are a part of human wisdom; for all their indeterminacy, they stand for something fundamental and inescapable.[4]

The oppositions I've chosen reflect the <u>life</u> of chemistry. And they gain strength through the subconcious associations we make of science and individual psychology.

It's no accident, I think, that there is a special pull on us, an archetypical feeling, to that classic of duality, Robert Louis Stevenson's "The Strange Case of Dr. Jekyll and Mr. Hyde". Hiding in that story is a critical chemical duality:

> My provision of the salt, which had never been renewed since the date of the first experiment, began to run low. I sent out for a fresh supply, and mixed the draught; the ebullition followed, and the first change of colour, not the second; I drank it, and it was without efficiency. You will learn from Poole how I have had London ransacked; it was in vain; and I am now persuaded that my first supply was impure, and that it was that unknown inpurity which lent efficacy to the draught.[5]

Avner Treinin is one of Israel's leading poets. And he is also a distinguished physical chemist. In an essay entitled "In Praise of Dualities" he writes:

> But probably the most compelling source of my attraction to science and poetry has been not the

similarities between them but rather the dissimilarities, even contradictions: to see the same thing from two apparently opposite perspectives and feel the mounting tension between the two.

There is something strange in our attitude toward contradictions. From childhood we are told to avoid them, to be consistent, while the whole of our experience teaches us not only that we are concentrated solutions of contradictions, but also that without them nothing could exist. Essentially, this is what dialectics is all about. The atom itself, the building block of all matter, is composed of positive and negative charges, and everything that flows (water, electricity, the pulses in my brain which are now composing this sentence), flows between opposite poles, that is, through a potential gradient. Moreover, from modern physics we learn that the only way to understand reality (if this can be called understanding) is to use two contradictory pictures which complement each other: particles and waves, or mass and energy...

So what is the wonder in finding that poetic and scientific pictures may complement each other in conveying to us some sense and essence of our existence, and that by bringing the two pictures together a powerful spark can be generated in the mind?

As any physical chemist dealing with surface phenomena knows, the important things happen at the boundaries between things, where something ends and something begins, like the tension created between adjacent poles, between body and soul, content and form, particles and waves, number and feeling. It is at the interface between two different media that light is reflected, refracted, converges, stimulates the optic nerve, forms the image — and we see.

In his notebooks, Leonardo da Vinci teaches his students how to paint the Deluge. After referring to many of its horrors, such as ships broken to pieces, flocks of sheep beaten on rock, hailstones, thunderbolts, whirlwinds, rotting corpes, and so on, he adds: "And if the heavy masses of ruin of large mountains or of other grand buildings fall into the vast pools of water, a great quantity will be flung into the air and its movement will be in a contrary direction to that of the object which struck the water, that is to say: the angle of reflection will be equal to the angle of incidence." Here is the confrontation between the "cold" physical law of reflection (the equality of angles) and the highly emotional description of death and destruction, between the concrete and the abstract, the general and the particular, the reproducible and the irreproducible, between order and chaos — between science and poetry.

> It is a very intense confrontation which strongly moves the soul. If dualities did not exist, we should have invented them, provided we could do it without any duality to begin with. This is probably the reason why God split Adam into two opposite poles. He wanted him to move, to be alive.[6]

And in a quite different context, the anthropologist Kathryn S. March concludes a paper on "Weaving, Writing, and Gender", in which she discusses the way weaving and Buddhist writing shape and are shaped by gender in the Tamang (a Tibetan origin group in north central Nepal), in the following way:

> Gender as a symbolic system specifically represents this very problematic or paradox, indeed, antinomy: to represent things that are, and are not, the same; things that might be the same if they were not interpreted from opposing perspectives; perspectives that emerge as opposed because they arise as women and men consider the gender logic of each other's position; men and women who, as they consider one another, confront the many ways in which they are, and are not, the same.[7]

1. The Pauli quotation is from Gerald Holton, "Analysis and Synthesis as Methodological Themata," in The scientific imagination: case studies, (Cambridge: Cambridge Univ. Press, 1978).

2. For an introduction to Hegel, see, F.C. Beiser, Ed., The Cambridge Companion to Hegel, (Cambridge: Cambridge Univ. Press, 1993), especially the chapter by Michael Forster on "Hegel's dialectical method," pp. 130-170.

3. There are "polypolar" epistemologies, one of the more intriguing of which is Mallarmé's, based on paradox. See R.G. Cohn, Modes of Art, Stanford French and Italian Studies, No. 1, (Saratoga, Calif: Anma Libri, 1975), esp. Ch. 1.

4. Emily R. Grosholz, "Nature and Culture in "The Souls of Black Folk and The Quest of the Silver Fleece," to be published.

5. Robert L. Stevenson, Dr. Jekyll & Mr. Hyde, the Merry Men and Other Tales, (London, J.M. Dent, 1925), p. 61. An article by David Jones reminded me of this episode.

6. Avner Treinin, "In Praise of Dualities", in Scopus 40 (1990): 54-56.

7. Kathryn S. March, "Weaving, Writing, and Gender", Man(N.S.) 18 (1983): 729-44.

CHEMISTRY TENSE, FULL OF LIFE?

Chemistry? The science which we notice only when a tank car of benzene finds itself in the river, and a town must be evacuated? Whose most exciting manifestation might be the fireworks on the 4th of July? Could this science be lively <u>and</u> intellectually deep?

Or is what I've done just a structural device, a trick? Take anything seemingly dull in this world, a day in a provincial accounting firm, a hard day cutting sugar cane in Cuba. Survey the limits which shape the middle, polarize, dichotomize, deconstruct all peaceful existence as a precarious struggle. If you're convincing enough, you can create tension where none was there before.

I don't think I've stirred up a Potemkin storm. Before there was science, the miracle of substances changing (today we would say "molecules reacting") had a most powerful hold on the human imagination. I refer to alchemy, a cross-cultural activity in which a philosophy of change was conjoined with proto-chemistry. With some charlatanry thrown in. Chemists would like to forget the esoteric philosophy, keep the proto-chemistry, and laugh at the charlatanry. But they were all tied firmly together.

The reason alchemy captured the imaginative faculties of people over centuries, across cultures, is that it touched something deep. Change (and stability) is physical and

psychical; juxtapose any two manifestations of change, and one immediately becomes a metaphor for the other.[1]

Goethe's novel, Elective Affinities", has been mentioned several times in this book. For good reason, for it is one of the few successful literary works taking off from a chemical theory. The idea of elective affinities, a theory soon superceded, was that certain chemical entities (we would now say molecular fragments) possess a special, definable, chemical affinity for each other. And yet, Goethe knew that he had done more than clothe a chemical theory in beautiful language. In an advertisement in Cotta's Morgenblatt he explained that the title of his book was a chemical metaphor, whose "Spiritual Origin" his novel would demonstrate.[2]

I think chemistry is interesting to its toiling practitioners, and to people who use it (or abuse it) without being chemists, because its activities parallel deep avenues in our psyche.[3] Which I prefer to see not as a branching tree of neurons, shaped by genetics, experience (and chance), but a completely interconnected multi-dimensional volume. In which a given fact (a molecule, a line from a poem) has a history, a context, to be sure. But it comes to life only if we think of the molecule (or the poem) as suspended — yes, tensely — in a space that is defined by different themes or oppositions.

In an imperfect metaphor, think of the themes as light of different frequencies. Or think of them as coordinate axes, not very linear, in a multidimensional space. I turn on the light of

identity, of the same-and-not-the-same, and I see cubane as different from other C_8H_8 molecules, many of which have been synthesized. I tune to the radiation of cooperation and competitiveness, and before me flashes the image of the Harvard Assistant Professor who once inspired me to do an overly simplistic calculation on cubane, a man who devoted years to making the molecule, and failed. Had he succeeded, he would have been promoted. I look at cubane in the multicolored light of utility and social responsibility, and I think about whether it should worry us that some of the work on it is supported by military research agencies, or that a derivative has been found to have antiviral activity, or that the strained molecule could find a use as a solar energy storage material.

The different ways in which any molecule is examined, where it falls not on one, but on many polarity scales make that molecule inherently interesting. The questions one asks the molecule touch silently, without our knowing it sometimes, on vital questions we should ask ourselves.

1. A fascinating perspective on alchemy is to be found in Mircea Eliade, The Forge and the Crucible, 2nd Ed, tr. Stephen Corrin, (Chicago: Univ. of Chicago Press, 1978).

2. R. J. Hollingdale, in the preface to his translation of Goethe's Elective Affinities, (Harmondsworth: Penguin, 1971), p.14.

3. On the psychological significance of alchemy, see C.G. Jung, Psychology and Alchemy, tr. R.F.C. Hull, (London: Routledge, 1953). For an introduction to Jung's work, see Storr, A., Jung, (New York: Routledge, 1991).

Chapter 51

CHEIRON

No less than four of the signs of the Zodiac are dualistic: Gemini, Libra, Pisces, and Sagittarius. I choose to see the constellations not as a vestige of dark ages, but as a timeless pointer to that irrepressible quality of the human soul that eventually led to science — curiosity, and a search for patterns.

Sagittarius is a Centaur. My favorite of these half man, half horse creatures of Greek myth is Cheiron. He was the son of Cronus (Zeus' father) and Philyra, the daughter of Oceanus.[1] Immortal Cheiron was sage and kind. From his cave on Mt. Pelion he taught the healing arts to Asclepius, the skills of riding, hunting, and pipe-playing to Achilles. He taught Diomedes, who became Jason of the Argonauts, he taught Aeneas. The teacher in me likes this teacher.

Good deeds (and no myth testifies to the contrary) did not bring Cheiron a happy old age. A bystander to a typical Centaur melee which was not his, he was wounded by a poisoned arrow (I wonder what poison?) fired by his friend Heracles. The great Centaur screamed in pain, but he could not die, for he was immortal. Finally Zeus granted him peace, in the process bringing about a significant conjunction of the wise Centaur who taught gods and men, and the rebellious Titan, Prometheus, who brought fire to humanity. Prometheus speaks, in the words of Aeschylus:

> Hear rather that all mortals suffered,
> Once they were fools. I gave them power to think.
> Through me they won their minds...
> Seeing they did not see, nor hearing hear.
> Like dreams they led a random life...
> From me they learned the stars that tell the seasons,
> their risings and their settings hard to mark.
> And number, that most excellent device,
> I taught to them, and letters joined in words.
> I gave to them the mother of all arts,
> hard working memory.[2]

For this Prometheus was punished, for teaching us to see. He was chained to a peak in the Caucasus, an eagle "feasting in fury on the blackened liver" of the of the Titan whose name means "forethought".

Hermes, Zeus' messenger, says to Prometheus

> Look for no ending to this agony
> Until a god will freely suffer for you
> Will take on him your pain, and in your stead
> Descend to where the sun is turned to darkness,
> The black depths of death.[3]

It was Cheiron who was willing to die for Prometheus. And in one of the greatest losses I feel we have suffered, the account of the subsequent reconciliation of Prometheus and Zeus, in the last part of Aeschylus' great trilogy, is missing.

So the fates of Prometheus and Cheiron intersected. The Centaur's name comes from the Greek word for hand, the same word that is at the root of that most subtle difference that may heal or kill, the nearly same, chirality. I imagine Cheiron stretching his hand out to Prometheus, as he gives him the gift of life.

As inherently good as Cheiron was, I do not want to romanticize the Centaurs, who were by and large a rough and

immoral bunch. But it is crystal-clear that Centaurs are the incarnation of the same and not the same. Man and beast, not whole human, not wild beast. Stationary and fleet, a tenser, complex, yet integrated being. Capable of harm, seeking for the good. Like chemistry.

ENDNOTES

1. R. Graves, The Greek Myths (Baltimore; Penguin, 1955), 151g. Some say he was the descendant of Nephele and Ixion (a thorn in Zeus' side), ibid, 63. The mythological information in this chapter derives from this source.

2. Aeschylus, Prometheus Bound, tr. E. Hamilton in Three Greek Plays (New York, W. W. Norton, 1975), p. 115.

3. Aeschylus, Prometheus Bound, in Hamilton, Three Greek Plays, p. 141.

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January 30, 1995

Professor Roald Hoffmann
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Dear Roald,

I am so sorry that you won't be able to be in Anaheim in April.

No, I don't know the painting Two Sisters by Theodore Chasseriau.

Thank you so much for sending me your essay and chapter of your book, which I really look forward to reading. I wonder whether you have loose copies of earlier drafts of some of your chapters; if so, I would love to read the chapter on Fritz Haber.

All good wishes.

Sincerely,