Alfred Bader fonds

Correspondence

Hargittai István + Magdolna

1995-2003

Subject: Nakanishi interview
From: Alfred Bader Fine Arts <baderfa@execpc.com>
Date: Fri, 03 Oct 2003 13:16:51 -0500
To: Professor Istvan Hargittai <hargittai.istvan@tki.aak.bme.hu>
CC: Arnold Thackray <athackray@chemheritage.org>, Frances Kohler <fkohler@chemicalheritage.org>

Dear Istvan,

When I saw the text of your complete intervie with Prof. Nakanishi, I was astounded and thought this your most exciting interview ever. When Arnold Thackray asked me whether this should be published I took counsel with a distinguished Lubavitch rabbi who agreed with me that this should be published.

Now I have just read the interview published in the latest Chemical Heritage news magazine, and I am deeply disappointed.

Historians should be tellers of the truth and not censors worried about political correctness.

What Nakanishi said is important. Not so much so about his comments about Palestinian terrorists which just show that he has not carefully considered the Israeli position. But his comments are most important for what he said about American complicity, as he sees it, in Pearl Harbor.

You and Chemical Heritage had the chance of publishing an astounding interview and you missed it.

Will you be able to publish the entire interview when this appears in your next book?

Best wishes,
Alfred Bader

Subject: Outrage and Sympathy
Date: Wed, 12 Sep 2001 08:47:22 -0700
From: "Hargittai, Istvan" <hargittai@tki.aak.bme.hu>
To: Bader Fine Arts <baderfa@execpc.com>

Dear Alfred:

Yesterday's events shook us and our thoughts are in the U.S.

Yours,

Istvan

Subject: Re: Cold Spring Harbor Laboratory
Date: Thu, 10 May 2001 10:04:17 -0700
From: "Hargittai, Istvan" <hargittai@tki.aak.bme.hu>
To: Bader Fine Arts <baderfa@execpc.com>

Dear Alfred:

I was most moved by the scope and focus of Daniel's Foundation and I would like to ask you to convey him my best wishes and admiration for his work.

With kind regards,

Istvan

==========
Prof. I. Hargittai
Budapest University of Technology
H-1521 Budapest, Hungary
P 36-1-463-4051, F -4052

Subject: Re: FYI/Copy/The Chemical Intelligencer
Date: Mon, 19 Jun 2000 11:59:47 +0200
From: Hargittai Istvan <hargittai.aak@chem.bme.hu>
To: baderfa@execpc.com

Dear Alfred:

I am saddened to inform you that Springer-Verlag New York has decided to cease publication of The Chemical Intelligencer with the last issue of Volume 6, at the end of the year 2000. I am now notifying all Editorial Board members and also all authors whose manuscripts are at various stages of the editorial process and production. We are having quite a backlog of unpublished manuscripts.

At this time I would like to thank you for your activities on behalf of The Chemical Intelligencer over the years. I hope that our fruitful and pleasant interactions will continue in the future.

With best wishes,

Istvan

==========

PS Just a little information about the schedule of my interview volumes that are now of added importance since many of my interviews will now appear only in these volumes.

I. Hargittai, Candid Science: Conversations with Famous Chemists. Imperial College Press, London, 2000 [this book has appeared, both in hardback and softback].

I. Hargittai, Candid Science: Conversations with Famous Biochemical Scientists. Imperial College Press, London [submission of manuscript for production at the end of 2000, to appear in 2001]

I. Hargittai, Candid Science: Conversations with Famous Physicists. Imperial College Press, London [submission of manuscript for production in the spring of 2001, to appear toward the end of 2001]

I. Hargittai, Candid Science: More Conversations with Famous Chemists. Imperial College Press, London [submission of manuscript for production at the end of 2001, to appear in 2002]

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Prof. I. Hargittai
Budapest University of Technology
H-1521 Budapest, Hungary
P 36-1-463-4051, F -4052

Subject: Re: Photograph
Date: Fri, 07 Jan 2000 09:11:29 +0100
From: Hargittai Istvan <hargittai.aak@chem.bme.hu>
To: baderfa@execpc.com

Dear Alfred:

Thank you very much for your gracious message. I am much concerned about the photograph.

Until yesterday I could have told you that mail does not get lost, alas, yesterday I received a small package from the U.S. and inside, there was only the packing material but not the thing that should have been in there. I am very disturbed. On the other hand, I receive a large amount of mail and sometimes with fancy stamps and I am not aware of things getting lost (except this upsetting case yesterday about which I at once initiated an investigation first at the post office and at the customs bureau, which is another great place where things go through). Unfortunately I cannot initiate any investigation about the lost photograph because there is nothing material I can base my request for an investigation on like in case of the package yesterday.

I wonder who has the negative of this image if it still exists. I know it is small consolation but Albert Eschenmoser has this photo too. I may have mentioned to you that I have recorded a conversation with Albert and he sent me this same photograph, among others, for illustrating the conversation.

I have returned the photos to Albert and hope they will arrive to him soon. I have not heard from him to this effect yet. Learning from some poor experience at Springer Production, I try to avoid sending them original art and I copied the photos on slides and retained a copy for myself too. In case you would like to use this same image, this slide is of very good quality and I can offer it to you. This lessens my being unhappy about the lost photograph but at least it is a possible replacement in case you would need it.

Magdi is joining me in sending you and Isabel our best wishes for 2000 and beyond.

Yours,

Istvan

At 13:05 2000.01.06. -0600, you wrote:
>Dear Istvan,
>
>Isabel and I have just returned from a long stay in Holland and England.
>
>Now I am sorry to note that the photograph of Woodward and Eschenmoser
>which I
>sent you by Air Mail on November 4th has gotten lost in the mails.
>
>Perhaps we made a mistake of putting such beautiful stamps onto the
>envelope; it
>may have tempted someone to steal it.
>
>With all good wishes for a happy and healthy new year I remain
>
>Yours sincerely,

>Alfred Bader
>
>Hargittai Istvan wrote:
>
>> Dear Mrs. Zuehlke:
>> I have not received the photo and my mail addressed to me is delivered to
>> me. Cheking with everyone at the Technical Univesrity, I don't quite know
>> what you mean by that, there are thousands of people here. One possibility
>> is if you did not mail it by Air then we can hope for its arrival later.
>> Kind regards,
>> Istvan Hargittai
>>
>> At 15:34 1999.12.17. -0600, you wrote:
>> >Dear Dr. Hargittai,
>> > We mailed the photograph to you on November 4th. It simply cannot be
>> >replaced. Please check with everyone at the technical university -- we
>> mailed it
>> >to:
>> >
>> >Professor Istvan Hargittai
>> >c/o Budapest Technical University
>> >Budapest, XI. SST.
>> >Gellért tér 4. H-1521
>> >HUNGARY
>> >
>> >Please keep us informed. Thank you.
>> >
>> >Sincerely,
>> >(Mrs.) Ann Zuehlke, Secretary
>> >
>> >
>> >Hargittai Istvan wrote:
>> >
>> >> To date I have not received the photograph.
>> >> IH
>> >>
>> >> At 13:48 1999.11.16. -0600, you wrote:
>> >> >Dear Dr. Hargittai,
>> >> >
>> >> >We sent the photograph to you by air mail the first week of November.
>> Just
>> >> >return it to Alfred when you receive it.
>> >> >
>> >> >Best regards,
>> >> >Ann
>> >> >
>> >> >Hargittai Istvan wrote:
>> >> >
>> >> >> Dear Alfred:
>> >> >>
>> >> >> A little more than two weeks ago we exchanged a couple of messages
>> about a
>> >> >> photograph from your book showing Woodward and Eschenmoser. At that
>> time
>> >> >> you were planning to send me that photograph. It has not come and I
>> >> >> presume that you did not send it to me. If this is the case, please,
>> don't
>> >> >> send it to me anymore bacuse in the meantime I have received it from
>> >> >> Eschenmoser himself. He included this photo among those he
offered to
>> >> >> choose some for using them to illustrate my conversation with him.
>> >> >>

>> >> >> I hope things are going well for you,
>> >> >>
>> >> >> Sincerely,
>> >> >>
>> >> >> Istvan
>> >> >>
>> >> >> ==
>> >> >> Prof. Dr. I. Hargittai
>> >> >> Budapest Technical University
>> >> >> H-1521 Budapest, Hungary
>> >> >> P 36-1-463-4051, F -4052
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>> >> >> Absences: Jan-March 2000, Cambridge, UK
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Prof. Dr. I. Hargittai
Budapest Technical University
H-1521 Budapest, Hungary
P 36-1-463-4051, F -4052

UNCW

THE UNIVERSITY OF NORTH CAROLINA AT WILMINGTON

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred: February 27, 1998

Many thanks for the corrections and for the added page on February 23. The printed versions have also arrived by mail. I am sending on to Springer-Verlag the corrections and the added page along with a few snapshots from my visit. The material is scheduled to appear in the July issue of *The Chemical Intelligencer*.

Many thanks again for your gracious cooperation in this matter.

With best wishes,

Yours sincerely,

Istvan Hargittai
Distinguished Visiting Professor
[on leave from Budapest until May 10, 1998]
hargittai@uncwil.edu
Fax 910-962-3013

DEPARTMENT OF CHEMISTRY

601 SOUTH COLLEGE ROAD · WILMINGTON, NORTH CAROLINA 28403-3297 · 910-962-3115 · FAX 910-962-3013

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

A Chemist Helping Chemists

February 24, 1998

To: Professor Istvan Hargittai
Fax: 910 / 962-3013

Dear Istvan:

Thank you so much for your fast response.

Of course, you are quite correct in pointing out that on page 5 of the 1995 interview, I mentioned that I divide my time three ways - one third buying and selling paintings, a second third working with chemical companies, and the last third writing and, of course, also giving many lectures. (I didn't mention the lectures in the interview, but surely that is not important.) Before 1995, we made some major gifts, such as, for instance, £6 million for Herstmonceux Castle and establishing chairs and awards in chemistry and art history. But that took relatively little time.

Now, we spend a good deal of time, probably about one-fourth, finding causes where we can really make a difference. These range from inner-city help in Milwaukee to many causes in the Czech Republic to far-lying problems such as the needy in Bulgaria and the traumatized in Bosnia. These now takes a great deal more time than it used to. My son, Daniel, heads the Helen Bader Foundation that gives away $8 million annually, but he has 12 competent people to help him. Isabel and I are doing this ourselves, and it really takes time. Even the simplest of gifts, such as the Project SEED scholarships of the ACS, require quite a bit of correspondence. If you would like me to send you more specific details - of course, on a confidential basis - I will be happy to fax these to you.

Isabel and I leave what we have to a foundation which will also by run by Daniel, but why shouldn't we enjoy giving quite a bit away while we are alive?

Please do let me know if I can send you some further information.

I very much look forward the publication of the interview in July.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Enclosure

Project SEED: A review and a call for volunteer mentors

Project SEED (Summer Educational Experience for the Economically Disadvantaged), a program supported by American Chemical Society members to provide a research experience in the chemical sciences for high school students from economically disadvantaged families, has undergone many changes in recent years. I want to provide a summary of the current program and its most recent evaluation, as well as a description of the role of SEED mentors—dedicated volunteers who host SEED students at their laboratories in academe, industry, or government. I hope that some of you will choose to participate in the SEED experience.

The major thrust of Project SEED is the summer research experience, a program now called SEED Summer I. In 1992, Alfred and Isabel Bader provided funds for an experimental program that would allow SEED students to participate in a second summer research experience, a program called SEED Summer II. The Baders were convinced that a second summer research experience for SEED students would enhance and be more productive than the first.

Another expansion of Project SEED occurred at about the same time, with the creation of college scholarships for former SEED students. It has been further enhanced by donations from Mettler-Toledo, Bayer, and Eli Lilly & Co. In 1998, the Project SEED scholarship program will continue to expand because of another generous gift from the Bader family. When matched by ACS, the Bader gift will provide an additional 20 scholarships.

Both the Summer I and Summer II programs have been reviewed, and the results have been gratifying (C&EN, Feb. 24, 1997, page 70). The C&EN article cited discusses the Project SEED Comprehensive (Summer I) evaluation; the Summer II evaluation, however, was completed after the article was published. I would like to summarize key points that emerged from that study. Students cited three reasons for wanting to participate in a second summer research experience—to improve skills and abilities in science, to develop interests in scientific/technical areas, and to earn money.

Herbert B. Silber
1997 chair
ACS Committee on Project SEED

Forty-nine percent of respondents rated the Summer II experience better than Summer I. Furthermore, 82% of respondents said Summer II provided a lasting stimulus for an interest in science. The impact of Project SEED Summer II appears to correspond well with the original goal of the program—giving high school students a better appreciation of work in science.

There will always be a need for member contributions so that Project SEED can maintain its size and, perhaps, even grow. In addition to the special funds received by Project SEED, the costs of the program are borne by the ACS Campaign for Chemistry/SEED endowment and from individual contributions from ACS members. In 1997, we ended a five-year period of reductions in the size of the SEED Summer I program that were necessitated by insufficient funds.

The second and most important component of a SEED summer program is to provide high school students with a good mentor, and currently, this is where we need the most help. The majority of SEED host sites are located in colleges, universities, medical schools and federal laboratories. We need to recruit more mentors from industrial laboratories to expose SEED students to the experience of work in the chemical industry.

With proper guidance, SEED high school students have been able to contribute significantly to a variety of research projects, and many have been coauthors of publications and patents. That many mentors return year after year to request SEED students for their laboratories is an indicator that they are very pleased with SEED students. Some students end up with further employment at the site of their SEED experience.

Many of us have served as mentors outside of work and family, such as time spent working with young people in our churches, temples, and mosques, or by being a little league coach. The fundamental aspects of these mentoring roles are to teach skills, teamwork, and respect for other members of the group. Being a mentor in the SEED program has many of the same aspects.

One of the first acts of a potential SEED mentor is to seek out SEED students and discuss a proposed research project. Many SEED students may have never met a scientist before. Moreover, because of the socioeconomic background of many SEED students, they need a stable person to talk to about life, school, and other issues. In addition to guiding students through a research project, a mentor listens and gives advice about future educational and career opportunities. The title of a recently published book on mentoring, "Adviser, Teacher, Role Model, Friend" (National Academy Press), summarizes how a student should feel about a good mentor.

If you are interested in becoming a Project SEED mentor, or if you would like to sponsor one or more SEED students, please call Project SEED at (202) 872-4380. We will be happy to provide more information.

Views expressed on this page are those of the author and not necessarily those of the committee

To Prof Adam Kanzigai

February 23, 1998

It is great fun - and instructive - to read what I wrote two-and-a-half years ago.

Fundamentally, nothing much has changed. Isabel and I now divide our time a little differently, namely four ways: working with small chemical companies - and actually being involved in the start-up of two - takes about one-fourth of our time.

Of course I am proud of the service that Sigma-Aldrich has provided to chemists, but I had really no idea quite how many friends we had among chemists worldwide. So I was staggered when I learned that I was elected one of the top 75 distinguished contributors to the Chemical Enterprise (C&EN, Jan. 12, 1998), a surprise sweetened by my friends at Aldrich congratulating me in an ad - as daring as kind.

My fine arts business has expanded considerably - the Rembrandt I bought in 1995 now hangs in a museum in Aachen, and just last month I bought another beautiful Rembrandt portrait and also an exciting Rubens, both at Sotheby's in New York. An excellent art historian and dealer in New York, Dr. Otto Naumann, handles most of the important sales, so I am more involved in finding than in selling great art. And I still find three or four great paintings a year for our own collection.

There are still many invitations to give lectures, both on the history of chemistry and art. I am particularly proud of my work on Josef Loschmidt, who is finally being recognized as a great chemist.

We now also spend more time, about one-fourth, helping people, both the ablest and the neediest through bursaries, scholarships, fellowships and awards. We are trying to improve our inner cities and to help the traumatized, for instance in Bosnia. Our biggest effort was to acquire Herstmonceux Castle for Queen's University. At first it created many problems for Queen's, but the International Study Centre is now running smoothly, and meeting hundreds of students there gives us such pleasure.

Our first granddaughter, Helena, is now three, and we are eagerly awaiting the arrival of two more grandchildren shortly. Time flies - but what a time it is when you watch your grandchildren. There is such a foolish saying: time is money - time is life that none of us can buy.

UNCW

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

A Chemist Helping Chemists

February 11, 1998

To: Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
The University of North Carolina at Wilmington
Fax: 910 / 962-3013

Dear Istvan:

Thank you for your fax of yesterday.

Rereading our conversation of November 8, 1995, I realize how very much has changed - all of it to the better - since then.

There are two alternatives:

(1) I can make a number of changes - not too many - so that you could date the conversation February 1998; or

(2) I can just write a couple of paragraphs to point out what has happened in the last two years.

With a competent secretary and a computer each of these would be easy.

Please let me know and I will reply within one week.

With all good wishes, as always,

AB/nik

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

A Chemist Helping Chemists

V Bader

To Prof. Istvan Hargittai

Corrected version

Best wishes

Alan

February 23, 1998

It is great fun - and instructive - to read what I wrote two-and-a-half years ago.

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

A Chemist Helping Chemists

February 23, 1998

Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
University of North Carolina
601 South College Road
Wilmington, NC 28403

Via: Mail (13 pages) and Facsimile (8 pages) 910 / 962-3013

Dear Istvan:

Thank you so much for your fax of February 11.

Enclosed please find my comments of today that I hope you will find satisfactory as an addendum to the November 8, 1995 interview.

I have looked at the eight pages of that interview and by and large it looks very satisfactory. You will note from the enclosed that I have made minor changes on pages 5, 7, and 8, and by fax I am sending you the corrected three pages as well as the original three pages. By mail I am sending you the entire interview with the corrections on the three pages interleaved.

To turn specifically to the corrections:

On page 5 I was chagrinned to see that I had misspelled Professor Haworth's name - even though Isabel and I have been in the building named after him many times.

On that page also I have added the brief note that we never bring very valuable paintings to Milwaukee.

On page 7 I have substituted the word *conservator* for the word restorer because conservators today do not really like being called restorers.

On page 8 I have just improved the English a little.

I very much hope that all this will be clear.

With all good wishes, I remain, yours sincerely,

AB/nik
Enclosures

February 23, 1998

a little differently,

It is great fun - and instructive - to read what I wrote two-and-a-half years ago.

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, about fourth,

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Alfred Bader
Milwaukee, Wisconsin, November 8, 1995

István Hargittai (IH): I would like to ask you about your chemistry. Not only did you create the famous company Aldrich, found *Aldrichimica Acta*, and build up a remarkable art collection, but you have also done considerable research in organic synthesis.

Alfred Bader (AB): I first became interested in research in my senior year as an undergraduate at Queen's University. There was a very good teacher, Professor Norman Jones, a famous spectroscopist. He allowed me to do a research project which I enjoyed. Then I got a very fine job with a paint company in Montreal, and a year and a half later the President of the company suggested that I go on with my studies and offered me company support. I did my Ph.D. studies at Harvard in 1947-1949 with Louis Fieser, who traveled so much at that time that his students saw very little of him. But there were many able chemists, students and faculty, who were very helpful.

Louis Fieser simply said to me, *'Here's a quinone; in alkali it turns red, overnight it turns yellow. Find out what happens.'* A year and a half later, he came into my lab and asked me *'How is that project going?'* I said I'd solved it. Fieser said *'Give a seminar.'* He was satisfied, said, *'write it up for a paper'*, and there it was. So all went well, but I realized one thing: I was not a world-class chemist. I was a very good experimentalist, but there were many things I didn't understand in theoretical chemistry.

I felt obligated to go back to the paint company in Montreal, but it had been bought by the Pittsburgh Plate Glass Co. whose paint research was concentrated in Milwaukee. So that is how I came here in January 1950. The company gave me a job but had no idea what to do with me. All the research they did was in oil chemistry - linseed oil, soybean oil - and here was a Ph.D. chemist from Harvard trained in synthetic chemistry. But they left me alone, and I got interested in producing monomers from inexpensive starting materials - phenol with butadiene, cyclopentadiene and isoprene, for instance. The literature said that chemists had tried the reactions and they didn't work. But I found that if I controlled the catalyst concentration carefully, I could make them work. We had a whole new series of unsaturated phenols, easily made from starting materials costing pennies.

One day a salesman from Quaker Oats stopped by and said that levulinic acid would soon be available very inexpensively from Quaker Oats. The moment I heard that, I made the bisphenol reacting levulinic acid with phenol to make what is now called diphenolic acid. A few weeks later, I sent a note off to JACS. Soon Johnson Wax wanted to buy the patent for which we had applied. Our Director of Research asked me, *'What should we charge for this?'* I said,

'It was two days' work; if we got ten thousand dollars, we would be well paid, but they must want it very badly, so ask for a million!' Well, he got it. Then, of course, lawyers descended on my lab to make sure everything I worked on was really patented, but I had already seen to that.

In 1954, PPG decided to move their paint research to Pittsburgh, but I didn't want to go there, left the paint company and devoted full time to Aldrich. Shortly after arriving in Milwaukee, I had asked my director of research whether he would allow me to start a small fine chemicals division. At that time, Eastman Kodak had a monopoly, but offered only 4,000 compounds. I thought we could easily make 250 compounds a year that were not in the Kodak Catalog. I was told that PPG was not interested; nobody could compete with Kodak. Yet today Kodak is no longer in the fine chemicals business. I felt that Kodak was not doing a good job and that chemists would be glad to have another source. So a lawyer friend and I set up a small company, Aldrich, very much a weekend operation with a capital of $500.

In the mid-1950's, when I visited customers, they would say, *'Aldrich, you're the cheap people.'* Kodak was very expensive, and they didn't really care about their fine chemicals business. They even had an ad in which they admitted that their service was poor. As a response, we published an ad saying *'Please bother us! We hope we never get so big that you can't talk to us.'*

IH: You've built up a library of chemicals. Where is it now?

AB: At Aldrich. It's close to a hundred thousand compounds. We have many famous chemists' research samples. For instance, Louis Fieser's, Bob Woodward's, Tadeus Reichstein's, you name them. A great many good things have come out of this library. Suppose that a medicinal chemist has an idea that a given bromolactone has some medicinal effect. He can contact Aldrich and get a computer printout of every bromolactone and order whichever he wants at $40 a sample.

Some years ago, a medicinal chemist in California, Dr. Summers, believed that acridines might help in the treatment of Alzheimer patients. He asked for our list of acridines, ordered some of each, and then came back wanting a hundred grams, then a kilo, then 10 kilos of one particular acridine. Years earlier, a Viennese chemist, Dr. Pickholz, working in London, had said to me, 'I've got this acridine, aminotetrahydroacridine; I think it's important in brain chemistry, I don't know how, but take a little, and we'll teach you how to make it'. For years, there was little interest in it until Dr. Summers came along. The rest is history: THA was, I believe, the first drug licensed by the FDA in the treatment of Alzheimer's disease.

IH: Should there be a universal library of all compounds?

AB: If there were a universal library, it would be run by some government agency, and it would be much more cumbersome to get samples. With Aldrich, it's very simple. It used to be called the Alfred Bader Library or the ABC Library, but when I was thrown out of the company, they dropped the Alfred Bader. Even ABC was too close; it's now called the Sigma-Aldrich Library, but it's still the same. Sales now exceed two million dollars a year, with many thousands of samples going out.

IH: What are the criteria for a compound to get into this library?

AB: It must not be in the Aldrich Catalog, and it must be clearly labeled. We don't analyze for the library, but we buy only from reputable researchers. Maybe two or three percent of the compounds are not what the researcher thought 20 or 30 years ago, and about 10% are not very pure.

IH: You said you didn't want to be so big. Why then did you merge with Sigma?

AB: It seemed to me in the late 60s, early 70s - but now I think I was mistaken - that organic chemistry had peaked. Woodward had synthesized strychnine; what more was there to do? This was before I really understood H.C. Brown's hydroboration. This was before Barry Sharpless' epoxidations. There's so much that has been done since. But I thought that most of the research funds would come to biochemistry and biomedical applications. I visited Sigma in St. Louis in the late 60's and proposed a merger, and they almost threw me out physically. Then Sigma went public in 1972, had some bad publicity and its stock dropped from 22 to 11. They were very thin in top management. At that point they listened to me, and the merger has been very good for everybody. Only Dan Broida, the head of Sigma, was against the merger. He was very dictatorial, but immensely hard-working, and you could call him day and night, collect. He had built Sigma sales to about 30 million dollars a year. Our combined sales then were about 45 million dollars. This year the sales of Sigma-Aldrich will be close to one billion dollars.

IH: You are still a stockholder; does it give you any say in company matters?

AB: I'm the largest individual stockholder, but it doesn't give me any say whatever.

IH: For decades you've been visiting synthetic chemistry laboratories in the best universities. Can you share some of your experiences with us?

AB: I don't see great differences among the countries where I used to go. Funding is very much more difficult in Britain than either in Germany or in the United States. The laboratories, the equipment are very much better in Germany and in the United States than in Britain. Comparing 1995 with 1950, a good chemist today could finish my Ph.D. work in a month. It took me a year and a half. There's so much more equipment around now. Then, NMR was unknown, and there was no mass spec. We had an infrared at Harvard, it was a big instrument and was on the blink 20% of the time, but it worked. It was amazing to listen to Bob Woodward or Gilbert Stork interpreting the spectra.

Today synthetic work can be done in so much smaller quantities than then. In our library of research chemicals, I can tell by looking at Woodward's students' bottles about when the compound was made. In the 1940s, 1950s, you had gram quantities; in the early 70s, you had hundred milligram quantities. Today 5 or 10 milligrams suffices.

IH: How about the image of chemistry?

AB: There has been a tremendous change, much for the worse. If you had gone to Harvard Square in 1947 and asked people on the street, *'What is your first reaction to chemistry?'*, they would have said, *'vitamins, new plastics, new drugs'*. Do it today and they answer, *'pollution and carcinogenic chemicals'*. We have not done a good job pointing out how much chemistry does. This is terrible - not for chemistry but for the world. When young, brilliant students see, for instance, the world sinking into a cesspool of toxic chemicals on the cover of *TIME* magazine, why should they want to become chemists? We rely on the media, and the media have done badly. I remember a headline in the *Milwaukee Journal* saying *"Benzene found in a well near chemical company"*. But the details in the text were that two parts per billion of benzene had been found. This is crazy. It's next to nothing. Our analytical ability has changed so that today we can show that everything is everywhere.

It's also true that there have been chemical industries that have done very wrong things, and then tried to hide them. The word *chemistry* has become an ugly word, but everything is chemical.

IH: About *Aldrichimica Acta*. To how many addresses is it delivered?

To be corrected

AB: It's free of charge, of course, and it goes to about 200,000 scientists worldwide. We have had very good papers in it. Over the years, we have established a number of awards in America, Canada, Britain and the Czech Republic. We used to ask the award winners to submit papers on their award addresses.

IH: Is there any connection between your collecting chemicals and collecting paintings of Old Masters?

AB: These are completely separate matters. Take the chemicals first. No chemist wants to throw out his research samples. Unfortunately, when a professor dies or retires, these are often discarded. I could tell you story after story. For instance, Professor Haworth's compounds at Birmingham. I feel so unhappy thinking about this every time I go to Birmingham. Here were thousands of his crystalline sugars, so difficult to crystalize. Some bureaucrat got worried, and they put many of these samples together into biscuit tins, poured in cement and threw them out. Imagine the idiocy of throwing out these crystals because some fool was afraid of these sugars!

Some years ago we went to Ames, Iowa, where all the Henry Gilman samples were stored in one big room, thousands of them. A company wanted $8,000 to remove them. I offered to pay for the chemicals and send a truck to pick them up. The only mistake we made was that the truck we sent wasn't big enough so we had to send it twice. There were 20,000 bottles. We immediately discarded about 12,000 because these were chemicals which Aldrich listed. There were another few thousand where the labels had fallen off or the materials had decomposed. We were still left with 3,000, and we published a little yellow catalog of the Gilman samples, just as we published a blue catalog of Woodward's samples.

About collecting paintings, when I was a kid, I lived in a home surrounded by paintings, but they were modern Austrian, and I didn't like them. In time, I realized that I liked Dutch historical paintings and Dutch portraits best. In the early 50s, I started buying pictures that I liked and that I could afford. Today I'm a dealer as well as a collector. I buy about 200 paintings a year. Last month I bought a very fine Rembrandt and yesterday I bought a beautiful TerBorch, probably the best outside of a museum. But I'm trying to have a non-elitist gallery. I have many pictures here from a hundred dollars up, and on the other hand, the Rembrandt is several million.X I spend about a third of my time buying and selling paintings, another third writing, and the remaining third working with chemical companies. I invest in them, consult and advise them. I'm trying to find customers for them and suggesting new products. I just bought a ten-percent interest in a large but very ailing English company called Anglo United, which owns Coalite. I know Coalite Chemical very well, and I think I may be able to help them.

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IH: Do you now do 100% what you like to do?

AB: Yes. I'm far happier today doing what I'm doing than I was four years ago. Then I had to work with the top management of Sigma-Aldrich in St. Louis. In the hundreds of meetings in hundreds of days in St. Louis, there was never a day that I really enjoyed myself there.

IH: What do you miss from those days?

AB: The most enjoyable part of my work was the 50% when Isabel and I simply walked from lab to lab, talking to students, asking them, *'What are you making that Aldrich should be offering? What do you need? What should we add to our catalog?'* My last such visit was early in 1992, before I was thrown out of the company, and I really miss those visits.

The most productive were to the top schools. We realized early on that 90% of the best research is done in 10% of the universities.

We would spend a most enjoyable day on the sixth floor of Chandler at Columbia University, for example, talking to each of the Gilbert Stork students, learning what they were doing and what they needed. Then a year or two later, I'd meet the same students as post-docs at the ETH or Cambridge, and two years later they'd have their first Assistant Professorship at an American university. It was a wonderful give-and-take. I was far better at that than I ever was as a research chemist.

IH: You give a great emphasis to your being Jewish in your autobiography. But you are Jewish by choice. You might have become Catholic, following your mother's side of your family.

AB: I was adopted by my father's sister, a Jewess. I also studied Judaism. At the time of the *Anschluß*, I was a boy of 14 in Vienna and saw all the propaganda of how terrible Jews were. I asked myself the question, *'What if these people are right?'* So I felt I had to study Judaism, and it became clear to me that the Nazis weren't right. I'm a convinced Jew and my two wives, Danny and Isabel, who came from religious Protestant backgrounds, became convinced Jewesses.

Coming back to the question about my Catholic mother, I hardly knew her. She would come once a month to the house, and occasionally she would say, *'Bobby [as I was called then], anyone who could be a Catholic and isn't is going to go to Hell.'* I didn't really know her as a person. I very much wanted to visit her in October of '47. She was then very sick and I asked Louis Fieser for three weeks off. *'No'*, he said, *'if you go, you'll lose your fellowship. Go next summer.'* Sadly, my mother died in April of '48.

To be corrected

IH: Referring to your two interests, what do you find common between chemistry and art?

AB: First of all, there is the restoration of paintings. This relies heavily on the knowledge of chemistry. Secondly, for hundreds of years, artists have tried to create something beautiful. Many artists today are desperately trying to create something new. They often use chemistry in their search for new materials.

People often ask me whether I restore my own paintings. I never do. When I buy a dirty old painting, I determine whether there is much nicotine on it. Often just saliva will take off a lot of dirt and nicotine. But I stop at that point and work with two very competent ~~restorer~~s. I have just acquired a painting which may be a late Rembrandt, with a terrible varnish. ~~The restorer will clean it and then~~ when it is cleaned we'll know better.

The ~~restorer~~s have to choose the right solvents, which usually take off the varnishes easily. The cleaning has to be done very carefully, and it may take a very long time. Often there is overpaint that has to be removed. Today we realize that all restoration should be reversible, but it wasn't so 200 years ago. Today competent ~~restorers do~~ inpainting is done over an easily removed varnish. Years ago, restorers often painted oil on oil. Almost all paints were based on linseed oil, which takes three or four hundred years to polymerize completely by oxidation. If a painting of the 16th century was overpainted in the 17th century, that overpaint has also polymerized and is very difficult to remove.

When I say overpaint, I'm not speaking of painting a new picture over another one. In the past, paintings were not so valuable, and possible damages and paint losses may have been corrected in an unprofessional manner. The restorers may just have been house painters, who overpainted much more than was needed. I have seen a little book, published in London in 1752, entitled *How To Be A Butler*. It advises that if the master has a dirty painting, the butler should take a bucket of wood alcohol (i.e. methanol) and a sponge. This would take off the dirt, but also the varnish and the top of the paint layer. There are so many paintings that have been skinned because the top layers have been removed.

I like nothing better than to find a 17th century painting to which nothing has been done. After 400 years, the polymerized paint film is practically indestructible, so the paint film holds the canvas together. But most paintings have been relined because over the years the canvas became as brittle as old paper. Restorers came along and backed the original canvas with a new canvas, putting glue in between. They'd put the painting face down, add a layer of glue, and the new canvas. Then they would use a hot iron to make sure that the new canvas adhered to the old. But when you do that to a thickly painted picture, the paint film gets flattened out, and this is terrible. Today, of course, competent restorers, if they have to reline, do it on a vacuum table so that the paint film doesn't get flattened out, but it is preferable to avoid relining

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To be corrected

altogether.

IH: What was the biggest mistake you made in the building of Aldrich and Sigma-Aldrich?

AB: We had some great chemists, ~~and~~ but I didn't treat them well enough financially, and they left.

We started the company in 1951 with a capital of $500, ~~our capital in 1951,~~ and I had to be penny-pinching. This was nothing new to me. I had never had any money, and even now I am still careful on a personal level. I realize that I should have been more generous with our best people.

IH: Was there any question in our conversation that you'd like to return to?

AB: Yes, concerning Aldrich. Clearly, my heart is with the company. I'm very proud of having founded Aldrich. Today research is different from the way it was in 1950 because Sigma-Aldrich supplies so many thousands of chemicals. We've made research very much easier and saved chemists of the world millions of hours that they can now devote to their own research rather than to making starting materials. I'm very proud of what I've done and of the many friends I've made around the world.

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UNCW

UNCW

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

A Chemist Helping Chemists

November 5, 1997

To: Professor Istvan Hargittai
Budapest Technical University
Fax: 36-1 463-4052

Dear Istvan:

Thank you so much for your letter of October 28th.

Of course we were so happy that Sir Harry won the Nobel prize, so very well deserved. We have seen him since and he is still the same exuberant and friendly man.

Of course there is no hurry whatever to your bringing out our conversation in *The Chemical Intelligencer*. All I could add now, five years after my expulsion from Sigma-Aldrich, is that I wear four hats. I divide my time between helping and consulting for all sorts of small and medium sized chemical companies, buying and selling about 200 paintings a year, writing and giving lots of lectures (see, for instance, the November issue of *Chemistry in Britain*), and trying to give money away intelligently. The fourth is the most difficult.

Would it be possible for you to send me what you plan to print? I promise you that I would make no changes whatsoever unless there is an actual, factual error. Knowing you, that is, of course, quite unlikely.

We will be in England, Scotland, and Spain from November 7th until December 18th and then back in Milwaukee.

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

AB/nik

Professor Istvan Hargittai
e-mail: hargittai@ch.bme.hu

Dear Istvan:

Please do not mind that I did not respond to your yesterday's fax immediately but I wanted to think about your question and discuss it with Isabel.

It seems to us that the three best places for you to study would be Philadelphia, Cornell University, and London.

I think that the Chemical Heritage Foundation headed by Arnold Thackray has a good many funds for visiting scholars, a very good library and excellent chemists nearby.

Roald Hoffmann at Cornell must have been charmed by your book on chirelity and surely you would really enjoy being at Cornell.

The Royal Institution in London is a very sleepy place with a great history, but probably very little funds. But University College, Imperial College, and King's College are nearby and one or the other of these may well have an opening.

I hope that I will live long enough to see your book of interviews. Should you reprint the one with me, please reverse the picture with my Mother's painting. Of course visually it does not really matter and I had to smile once again thinking of your great book about chirality.

A great art historian once said to me that the way to determine whether a painting is an original is to look at it in reverse. If it still looks good in reverse, it is an original. Of course I know that Mother's painting is the original. Before she was sent to Theresienstadt, she rolled up this and two other family portraits and left them with the painter who kindly gave them to me in 1949.

With all good wishes, as always,

Subject: Greetings from Budapest
Date: Thu, 13 Aug 1998 16:32:04 +0200
From: Istvan Hargittai <hargittai.aak@chem.bme.hu>
To: baderfa@execpc.com

Dear Alfred:

I was happy to receive your e-mail message. I didn't know you had e-mail. This makes communication much easier and inexpensive.

About the interview: I wanted to thank you for the interview. I enjoyed working on it and special thanks for your having taken the trouble to prepare the addition. I think your portrait conveys some of the warmth you have, at least others have agreed with me on this. You may remember I took this picture in front of your home. Unfortunately the other two pictures appeared more pale in printing than they actually are, but they still convey the atmosphere of your home too.

Magdi and I are spending our summer at home. Our daughter, Eszter, was here for a very brief visit. She is a grad student (sociology, internet) at Princeton. Our son, Balazs, is coming next week for a couple of weeks. He is a grad student in peptide chemistry at Minneapolis and will be attending the European peptide meeting in Budapest. Hopefully he will be finishing next year. He is already starting looking for a postdoctoral position.

There is something I would like to ask you for advice at this time. I am increasingly more and more fascinated with general questions of the progress of chemistry and by the lessons my interviewees teach us. I have continued collecting the interviews and have now over 80 and almost half of them Nobel laureates. I know it is not the only criterium of greatness but still it signifies the level of the collection.

I would like to work on a book of these lessons. In a way I like to think that what may come out of it might be a very incomplete and subjective but yet interesting panorama of 20th century chemistry. But there are less conspicuous lessons that are also important, and may even be more important. For example, the transferability of knowledge. Many great scientists have become what they are not so much for the amount of knowledge they had than for their ability to transform their knowledge from one field to another.

What I am lacking here is good library facilities and interactions with people. We are planning to spend one more semester, next spring, at the University of North Carolina at Wilmington, but that is not what I would like to have for this project either.

I would like to ask for your advice as to how to achieve the following dream. I would like to spend two semesters, not necessarily continuously the two semesters and not necessarily in the same place, in good universities (I have in mind British, Canadian, or U.S.) where I could be using the university facilities and interact with colleagues and work primarily on the book.

I would be happy to do some teaching and I am a good teacher, and could offer either a service course, general chemistry (1), or some speciality course, like symmetry (2), or something related to the book under work, like Reflections on 20th Century Chemistry (3). The first could be used for any introductory chemistry and I have had a lot of practice in teaching that in the U.S. The second could be suitable for a very broad spectrum of students, or, for example, as a science course for non-science majors, and I have had some experience in it. The third might be very useful for

seniors and grad students in chemistry to provide them an overview in our overspecialized world.

Alfred, as I am writing this message I am getting carried away, so I hope you will excuse my verbosity.

I can take a leave from my university in Budapest, especially if it is one semester at a time. These leaves are without pay, so I would need some support for subsistance but I see a problem also in getting myself accepted by a good school and being given the logistics needed in this unusual project.

Since we are planning one last semester in North Carolina in the spring of 1999, what I am looking for is for 2000 and beyond, and I would appreciate any advice, comment, or even sobering thoughts if you think my dreams are too far-fetched.

If you have read this letter this far, I thank you for it because even compiling this letter gave me a good feeling.

With best wishes also to Isabel and also on Magdi's behalf,

Istvan
Dr. I. Hargittai, Professor of Chemistry
Budapest Technical University, H-1521 Budapest
P 36-1-463-4051, F -4052

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4051, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred: October 28, 1997

I trust that both of you are doing well. Last year it must have been a great moment for you too when the Nobel Prize was announced for Harry. We were very happy to hear that news too. Magdi and I were in Stockholm those days.

I am sorry it is taking so long to bring out our conversation in *The Chemical Intelligencer*. However, it is in the pipeline. At this time I would like to ask you whether there is anything that you think should be added in view of the time that has elapsed since we had recorded it.

With best wishes,

Yours sincerely,

Istvan Hargittai

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

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

A Chemist Helping Chemists

September 20, 1996

Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
University of North Carolina
601 South College Road
Wilmington, NC 28403

Dear Istvan:

Thank you so much for your letter of September 2nd.

Setting a deadline for the simple correction of a manuscript by year-end certainly makes it very easy, and I demand a good more of myself!

The corrected transcript of our conversation is enclosed. You will note that I have added one more question - about the most serious mistake I ever made - towards the end and otherwise just made some factual corrections and corrections of English. I do hope that you will find this satisfactory.

As you will have realized, I am most anxious to see Professor Buchan's paper in *The Chemical Intelligencer*. Will it be in the October issue?

Is there any chance that you might visit us in Milwaukee before long? We plan to leave for England on November 8th and stay there until early January. But then, except for an ACS tour here and there, we will be in Milwaukee until the middle of March.

With all good wishes to you and Magdi, I remain,

Yours sincerely,

AB/cw
Enclosures

UNCW

THE UNIVERSITY OF NORTH CAROLINA AT WILMINGTON

September 2, 1996

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred:

Thank you very much for your kind letter of August 5. I am catching up with all my correspondence amid the beginning of the academic year here and everything else starting at the same time.

First of all, many thanks for your finalized manuscript on Loschmidt. I truly appreciate your patience and kind cooperation in this matter. This piece seems to be now in perfect order and I will be sending it to Springer for production with the next batch of material in about 10 days time. My tardiness in responding you has no influence on the publication schedule which will be slow in any case because of the backlog of manuscripts. However, at least the manuscript will be in the production pipeline. Springer has taken care of stamps and other valuable originals with great care and I only need to ask you for more patience in expecting back your originals as this is very slow indeed.

Concerning the transcripts of our conversation, I hope you won't be changing its conversational style so that it reads as a live conversation indeed. There is no haste about correcting them and I am fully aware of your having many more pressing matters especially after such a long absence from your office. I don't want to be a nuisance by setting deadlines but I wonder if you would find it comfortable to check the transcripts before the year is out?

With best wishes to both of you, also from Magdi who this week is in Norway refereeing a PhD Dissertation.

Yours sincerely,

DEPARTMENT OF CHEMISTRY

601 SOUTH COLLEGE ROAD · WILMINGTON, NORTH CAROLINA 28403-3297 · 910-962-3450 · FAX 910-962-3013

Symmetry through the Eyes of a Chemist

Second Edition

by István Hargittai, *Budapest Technical University and Hungarian Academy of Sciences, Budapest,* **and Magdolna Hargittai,** *Hungarian Academy of Sciences, Budapest*

From reviews of the First Edition:

*"**A fascinating overview** of the rich variety of applications of symmetry throughout chemistry, showing both its power and its aesthetic appeal."*

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—Journal of the American Chemical Society

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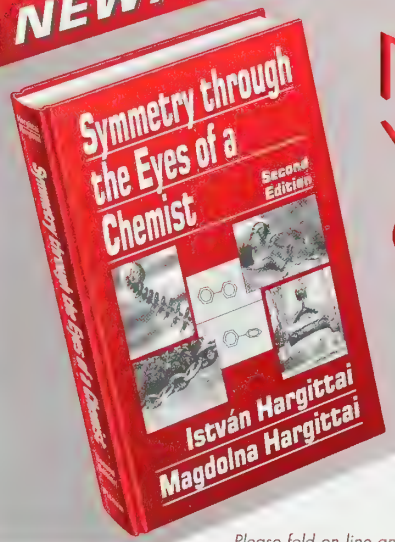

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2961 North Shepard Avenue
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A Chemist Helping Chemists

August 25, 1995

Via Facsimile: 36-1-463-4052 and Mail

Professor Dr. Istvan Hargittai
Professor of Chemistry
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Professor Dr. Hargittai:

Thank you for your letter of August 14th, received only today because you sent it by registered mail. That always delays mail.

My autobiography was published by Weidenfeld & Nicolson, Orion House, 5 Upper St. Martin's Lane, London WC2H 9EA, England, and the book's ISBN number is 0-297-83461-4.

I despair of your getting the book easily from Weidenfeld sent to Budapest. They are very competent publishers and very incompetent distributors; they even have difficulties distributing the book, which was printed in England, to English booksellers.

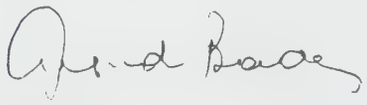
I presume that sometime before coming to Milwaukee, you can be reached in the United States, and if you will give me your forwarding address and let me know when you will be there, I will send you a copy of the book and also detailed directions to get to my office. As we are in the center of Milwaukee and close to the expressway from Chicago, you will not have much difficulty finding me. The drive from the center of Chicago to my office takes about two hours, unless there happen to be long delays in downtown Chicago.

Thank you for sending me the third issue of The Chemical Intelligencer, which I like very much. David Walton at the University of Sussex is one of my oldest friends in England. Is there some way in which I could acquire the first and second issues and then subscribe?

I very much look forward to meeting you and Mrs. Hargittai on November 9th.

With all good wishes, I remain,

Yours sincerely,



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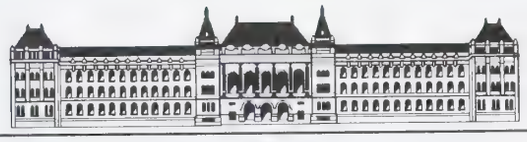

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4041, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

August 14, 1995

Dr. Alfred Bader
2961 North Shephard Avenue
Milwaukee, WI 53211

Dear Dr. Bader:

Thank you very much for your kind letter of August 1. I am very pleased that you are willing to participate in this project. My preference is also November 9 so this is very good. If it's convenient for you, I would like to tape our conversation in the morning and would be happy to accept your invitation for lunch.

I shall be travelling with my wife, a fellow chemist, and we shall be using a rented car. The previous evening we'll probably be staying somewhere on the road between Chicago and Milwaukee and I would like to get as detailed directions to our meeting place as you find it useful. I am not a too experienced driver and we have never been in Milwaukee before.

Thank you very much for alerting me to your book, *Adventures of a Chemist Collector*. I would like to get the Publisher's address because I would like to ask them to send me a review copy. Under normal circumstances I would like to buy a copy right away but it is still rather complicated and time-consuming here to buy a book from Britain. Not at all impossible but not trivial either. Since I would very much like to read the book before we meet, I wonder if you could have a copy sent to me as this seems to me the most direct, though not the most polite way on my part, to make sure I read the book in time.

As for The Chemical Intelligencer, its third issue just appeared and I am sending you a sample copy under separate cover. I hope you'll like this magazine. I certainly enjoy doing this project. It has also occurred to me that as much as I find it useful to read your book before we meet, I should probably provide some information about myself for you. So I am enclosing a recent Vita.

I shall be very much looking forward to our meeting on November 9,

Yours sincerely,

Istvan Hargittai

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

István Hargittai

Place and date of birth: Budapest, August 11, 1941

Parents: Magdolna Brünner (1908-1988), Jenô Wilhelm (1901-1942)

Education, degrees:
Eötvös University , Budapest, 1959-1961
Moscow University, Moscow, 1961-1965, Master's degree in chemistry 1965
Hungarian Academy of Sciences (HAS), Budapest, Candidate of Science 1971
Eötvös University, Budapest, Dr. rer. nat. 1972
Hungarian Academy of Sciences, Doctor of Science 1976
Corresponding Member, Hungarian Academy of Sciences, 1987
Foreign Member, Norwegian Academy of Science and Letters, 1988
Dr. honoris causa, Moscow University, 1992
Full Member, Hungarian Academy of Sciences, 1993
Member, Academia Europaea, 1994

Career summary:
Research Scientist, Center for Studies on Chemical Structures, HAS, 1965-1973
Visiting Scientist, Chemistry Institute, University of Oslo, 1968, 1975, 1981
Research Associate, Department of Physics, University of Texas, Austin, 1969/1970
Research Scientist, 1973-1975, Senior Research Scientist, 1975-76, Central Research Institute of Chemistry, HAS
Head of Department of Electron Diffraction & Quantum Chemistry, Central Research Institute of Chemistry, HAS, 1976-1979
Head of Department of Structural Studies, Research Laboratory for Inorganic Chemistry, HAS, 1979-1986
Science Advisor (HAS), 1982-1993
Visiting Professor of Physics, University of Connecticut, Storrs, 1983/1984
Visiting Professor of Chemistry, University of Connecticut, Storrs, 1984/1985
Visiting Professor of Chemistry, University of Texas, Austin, 1986/1987
Visiting Professor of Chemistry, University of Connecticut, Storrs, 1988/89
Visiting Professor of Chemistry, University of Texas, Austin, Summer 1989
Visiting Professor of Chemistry, University of Hawaii, Honolulu, Fall 1989
Visiting Professor of Chemistry, University of Hawaii, Honolulu, Spring 1993

Current positions:
University Professor, 1991- and Head of Institute of General and Analytical Chemistry, Budapest Technical University, 1991-
Research Professor, 1993- and Head of Department, Structural Chemistry Research Group, HAS, Eötvös University, 1986-

Career-related activities:
Title of Associate Professor, Eötvös University, 1975, Title of Professor, Eötvös University, 1980
Principal Investigator, HAS-University of Texas joint molecular structure research project, 1973-1977
Member, Directors' Council, Central Research Institute of Chemistry, HAS, 1976-1979

Consultant, Sektion für Strukturdokumentation, Universität Ulm, 1977-1992
Scientific director, International Summer School "Diffraction Studies on Non-Crystalline Substances", Pecs, Hungary, 1978
Consultant, Commission on Electron Diffraction, International Union of Crystallography, 1979-1981
Co-director, International School of Crystallography, 11th Course, Static and Dynamic Implications of Precise Structural Information, Erice, Italy, 1985
Head of Ph.D. Program in Inorganic Chemistry and Applied Chemical Research, Budapest Technical University, 1993-
Chair, Program Committee, Quasicrystals International School, Eötvös Physical Society, 1995

Editorial activities, Periodicals:
Editor, Structural Chemistry (Plenum Press, New York)
Editor-in-Chief, The Chemical Intelligencer (Springer, New York)
Editor, Advances in Molecular Structure Research (JAI, Greenwich, CT)
Advisory Board, Methods in Stereochemical Analysis (VCH, New York)
Editorial Board, Speculations in Science and Technology (London)
Editorial Board, Computers & Mathematics with Applications (Pergamon Press, Oxford)
Editorial Advisor, Leonardo (MIT Press, Cambridge, MA)
Editorial Board, A kémia újabb eredményei (HAS, Budapest)
Editorial Board, Kémiai Közlemények (HAS, Budapest)
Advisory Board, ACH – Models in Chemistry (HAS, Budapest)
Editorial Board, Journal of Biological Systems (World Scientific, Singapore)
Editorial Board, Fullerene Science and Technology (Dekker, New York)

Professional and association memberships:
Member, Commission of Electron Diffraction, International Union of Crystallography, 1981-1990
Member, Hungarian National Committee of the International Union of Crystallography
Member, Hungarian National Committee of CODATA, 1978-1985
Member, Advisory Board of the Austin Symposia on Molecular Structure, 1992-
Member, UNESCO, Hungarian National Committee, 1992-
Chairman, Task Group on Gas-Phase Structural Data, Hungarian National Committee of CODATA, 1981-1985
Member, Sigma Xi, The Scientific Research Society (USA), 1984
Chairman, Committee on Physical Chemistry and Inorganic Chemistry, HAS, 1990-1996
Chairman, Michael Polanyi Prize Award Committee, HAS, 1992-1996
Member, Hungarian Chemical Society
Member, Lorand Eötvös Physical Society
Member, International Group for Correlation Analysis in Chemistry
Member, American Association of University Professors, 1983-85, 1988-89
Member, Institute of Materials Science, University of Connecticut, 1983/1985, 1988/89
Member, International Advisory Board, Earth Sustainability Foundation (Vancouver)
Honorary Member, International Symmetry Society, 1992
Member, American Chemical Society, 1985
Foreign Member, Japan Institute of Hyperspace Science, 1992
Member, The New York Academy of Sciences, 1987
Member, Scientists' Club, HAS

Awards, etc.:
Academy prize for authors, Budapest, 1977
Academy prize for book critics, Budapest, 1979
Hassel Lectureship, University of Oslo, 1981
Torok Lectureship, University of Arkansas, 1986
Best Journal Issue Award by the Association of American Publishers, 1986
Joint Research Award of the Hungarian and Soviet Academies of Sciences, 1988
Dozor Visiting Professor, Israel, 1991
Japan Society for the Promotion of Science, Visiting Professor, 1992
Presentation and Introduction to the Academy of Sciences, Institut de France, Paris, 1993
Kaskan Lectureship, State University of New York at Binghamton, 1994
The Japan Academy, Visiting Professor, 1994
The Royal Society, Visiting Professor, Birkbeck College, London, 1994

Invited lectureships to international meetings include:
Current Research in Crystallography, Manchester, 1971
Fourth European Conference on Microwave Spectroscopy, Tübingen, 1977
Seventh Austin Symposium on Gas-Phase Molecular Structure, 1978
Eighth European Crystallography Meeting, Liege, 1983
Tenth Austin Symposium on Molecular Structure, 1984
Symmetry Symposium, Darmstadt, 1986
Quantum Theory and Experiment Applied to Solids, College Park, MD, 1986
Shubnikov Centennial Meeting, Moscow, 1987
Z. phys. Chemie Centennial Meeting, Leipzig, 1987
Art and Technology Conference, Lisbon, 1987
Twelfth Austin Symposium on Molecular Structure, 1988 (Banquet speaker)
9th IUPAC Conference on Physical Organic Chemistry, Regensburg, 1988
Fourteenth Austin Symposium on Molecular Structure, 1992
Art and Mathematics Conference, Albany, NY, 1992
NATO Advanced Research Workshop: Structures and Conformations of Non-rigid Molecules, Ulm, 1992
22nd Congress of the Italian Crystallographic Association, L'Aquila, 1992
Fifth European Meeting of Gas Electron Diffraction, Blaubeuern, 1993
Current Trends in Computational Chemistry, Jackson, MS, 1993
14th International Symposium of Fluorine Chemistry, Yokohama, 1994
1st World Congress of Transdisciplinarity, Setubal, Portugal, 1994
Current Trends in Computational Chemistry, Jackson, MS, 1994 (Banquet speaker)
NATO Advanced Study Institute: Large Clusters of Atoms and Molecules, Erice, Italy, 1995

Visits, invited lectures:
Austria, Belgium, Canada, China (PR), Czechoslovakia, Denmark, the Federal Republic of Germany, France, the German Democratic Republic, Great Britain, Italy, Israel, Japan, Korea (Republic of), Liechtenstein, the Netherlands, Norway, Poland, Portugal, Romania, Russia, Spain, Switzerland, U.S.A., U.S.S.R.

Invited seminars include:
Charles University (Prague), Moscow University, Soviet Academy of Sciences (Moscow), D.D.R. Academy of Sciences (Berlin), The Hebrew University (Jerusalem), Technion (Haifa), The Weizmann Institute (Rehovot), Technical University of Bucharest, Argonne National Laboratory (Argonne, IL), Naval Research Laboratory (Washington, DC), Cornell University (Ithaca, NY), University of Florida (Gainesville), University of Pennsylvania (Philadelphia), Smith College (Northampton, MA), Birkbeck College (London), University of Manchester Institute of Technology, University of Edinburgh, McMaster University (Hamilton, Ont.), Polish Academy of Sciences (Warsaw), Rocasolano Institute of Physical Chemistry (Madrid), University of Granada, University of Leiden, University of Leuven, University of Frankfurt, University of Münster, German Chemical Society (Göttingen), University of Ulm, University of Trondheim, Oregon State University (Corvallis), IBM T.J. Watson Research Center (Yorktown Heights, NY), University of Bern, University of Fribourg, University of Lausanne, ETH Physics Institute (Zürich), Solid State Research Institute of the Max-Planck-Gesellschaft (Stuttgart), University of Rome, University of Milan, CNR Structural Chemistry Laboratory (Montelibretti), Tokyo University, Ochanomizu University (Tokyo), Institute for Molecular Science (Okazaki), Kyushu University (Fukuoka), Hokkaido University (Sapporo), Seoul National University, Korea Advanced Institute of Science and Technology (Taejon), University of Paris (Orsay), Pasteur University (Strasbourg), University of Bologna, University of Wiscosin (Madison), Northwestern University (Evanston, IL), University of Vienna, Technical University of Vienna, Toyohashi University of Technology, Kobe University, University of Sussex (Brighton), National Science Foundation (Washington, D.C.), U.S. Army Research Lab. (Aberdeen Proving Ground, MD), Georgetown University (Washington, D.C.), University of Maryland (College Park), Technical University (Berlin), University of Göttingen, University of Essen, ETH Chemistry Institute (Zürich), New York University.

Research interest:
Structural chemistry; sulfur and silicon stereochemistry; coordination compounds; metal halides; unstable species; high-temperature chemistry; gas-phase electron diffraction; combined use of experimental techniques and theoretical chemistry; gas/solid structure differences; intramolecular and intermolecular interactions; models of molecular geometry; general problems of symmetry.

Teaching interest and experience:
Graduate-level teaching on molecular structure, electron scattering (Budapest, since 1971)
Third-cycle lecturer in Swiss French Universities, Bern, Fribourg, Lausanne, 1991
Graduate course teaching, Ben-Gurion University, Beer Sheva, Israel, 1991
General chemistry and general physics (U.S.A., 1983, 84, 85, 86, 87, 88, 89, 93)
Symmetry course for biology majors, University of L'Aquila, L'Aquila, Italy, 1994
Symmetry (interdisciplinary audiences)
Master theses advisor, Eötvös University
Dr. rer. nat. theses advisor, Eötvös University
Ph. D. theses advisor, Budapest Technical University

Authored books include:

The Electron Diffraction Interatomic Distance (in Hungarian), Akademiai Kiado, Budapest, 1974

The Molecular Geometries of Coordination Compounds in the Vapour Phase (with M. Hargittai), Elsevier, Amsterdam, New York, 1977 (Russian translation, MIR, Moscow, 1976)

Sulphone Molecular Structures. Lecture Notes in Chemistry, Vol. 6, Springer-Verlag, Berlin, Heidelberg, New York, 1978

The Structure of Volatile Sulphur Compounds, Reidel, Publ. Co., Dordrecht, Boston, Lancaster, 1985 (Russian translation, Nauka, Moscow, 1986)

Symmetry through the Eyes of a Chemist (with M. Hargittai), VCH Weinheim, 1986; Paperback edition: VCH Publishers, New York, 1987 (Russian translation, MIR, Moscow, 1989). Second, revised edition, 1995 (Plenum Press, New York)

Discover Symmetry (in Hungarian, for children, with M. Hargittai), Tankönyvkiadó, Budapest, 1989

The VSEPR Model of Molecular Geometry (with R.J. Gillespie), Allyn & Bacon, Boston, 1991 (Russian translation, MIR, Moscow, 1992; Italian translation, Zanichelli, Bologna, 1994)

Symmetry: A Unifying Concept (with M. Hargittai), Shelter Publications, Bolinas, CA, 1994

Edited books:

Diffraction Studies on Non-Crystalline Substances (with W.J. Orville-Thomas), Elsevier, Amsterdam, New York, 1981

Symmetry: Unifying Human Understanding, Pergamon Press, Oxford, 1986

Stereochemical Applications of Gas-Phase Electron Diffraction (with M. Hargittai), Vol. A: *The Electron Diffraction Technique.* Vol. B: *Structural Information for Selected Classes of Compounds.* VCH Publishers, New York, 1988

Crystal Symmetries, Shubnikov Centennial Papers (with B.K. Vainshtein). Pergamon Press, Oxford, 1988

Symmetry 2: Unifying Human Understanding, Pergamon Press, Oxford, 1989

Quasicrystals, Networks, and Molecules of Fivefold Symmetry, VCH, New York, 1990

Accurate Molecular Structures (with A. Domenicano). Oxford University Press, Oxford, 1992 (Russian translation, MIR, Moscow, in press, 1995)

Fivefold Symmetry, World Scientific, Singapore, 1992

Spiral Symmetry (with C.A. Pickover), World Scientific, Singapore, 1992

Advances in Molecular Structure Research, Vol. 1 (with M. Hargittai), JAI Press, Greenwich, CT, in production, Vol. 2 in preparation.

Combustion Efficiency and Air Quality (with T. Vidóczy), Plenum Press, New York, 1995

Edited journal issue:

Molecular Crystal Chemistry (A. I. Kitaigorodskii Memorial Issue, with A. Kalman), ACH - Models in Chemistry, 1993

Book chapters: over 15, **Review articles:** over 12, **Scientific papers:** over 200, Reports, popular articles, etc.

Posters:
Symmetry in Nature (with M. Hargittai), Tarquin Publ., Diss, U.K., 1995
Symmetry in Cities (with M. Hargittai), Tarquin Publ., Diss, U.K., 1995

Married:
1967, Dr. Magdolna Hargittai (née Vámhidy), D. Sc., Science Advisor, Hungarian Academy of Sciences

Children:
Balazs (1970), M.Sc. Chemistry (Eötvös University 1993), Ph. D. student, Northwestern University (Evanston, IL)
Eszter (1973), student, Smith College (Northampton, MA)

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Phone: (36-1) 463-4051, Fax: (36-1) 463-4052
e-mail: hargittai@ch.bme.hu
Structural Chemistry Research Group, HAS, Eötvös University, Puskin utca 11-13, H-1088 Budapest, Hungary
Mailing address: Pf. 117, H-1431, Budapest, Hungary
Phone: (36-1) 266-3722, Fax: (36-1) 266-3899
e-mail: h2399har@huella.bitnet
Home: Mandula utca 25, H-1025 Budapest, Hungary, Phone: (36-1) 135-8659

January, 1995

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

A Chemist Helping Chemists

August 1, 1995

Dr. Istvan Hargittai
Professor of Chemistry
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Dr. Hargittai:

Thank you so much for your letter of July 14th.

I very much look forward to meeting you and both November 9th and 11th would be fine, though I would much prefer Thursday, November 9th, which to me is completely open. On Saturday, November 11th, I could see you only in the afternoon, say between 3:00 and 5:00 p.m.

If convenient to you, I would also like to invite you either for dinner or lunch on Thursday or for dinner on Saturday.

Before your visit, you might like to glance at my autobiography, *Adventures of a Chemist Collector*, of which I enclose a review published in *Chemistry in Britain*.

Much looking forward to meeting you, I remain,

Yours sincerely,

AB/cw

Enclosure

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4041, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

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

July 14, 1995

Dear Dr. Bader:

In November I am planning a visit in the US, and using this opportunity, I would like to come and visit you and record a conversation with you for our new magazine The Chemical Intelligencer, of which I am Editor-in-Chief.

The Chemical Intelligencer is published by Springer-Verlag New York and it is an informative and entertaining magazine for chemists and related professionals. It is a quarterly. I am enclosing a reprint from the second issue. This reprint is of a set of interviews that I recorded last year with Professors Kenichi Fukui in Kyoto and Roald Hoffmann in Budapest.

If it would be convenient for you, I would like to come to see you late morning or in the afternoon of Saturday, November 11. I'll probably be driving early in the morning of that day from Chicago, and drive back to Chicago after our meeting. If you could spare me about an hour that would be wonderful but I won't be much limited in time in case you have a little more time for our conversation. An alternative day could be November 9, Thursday.

I would be delighted if you'd find to have such a meeting possible, and would appreciate hearing from you to this effect.

Thank you.

Yours sincerely,

Istvan Hargittai

Budapest, XI. SST. Gellért tér 4. H-1521, Hungary

Fukui and Hoffmann

Two Conversations

ISTVÁN HARGITTAI

Kenichi Fukui (b. 1918) is currently Director of the Institute for Fundamental Chemistry in Kyoto, Japan.

Roald Hoffmann (b. 1937) is currently Newman Professor of Physical Science, Department of Chemistry, Cornell University, Ithaca, New York.

Professors Fukui and Hoffmann were corecipients of the Nobel Prize in chemistry in 1981 "for their theories, developed independently, concerning the course of chemical reactions."

The two conversations took place within a few weeks' time in the Summer of 1994. The circumstances though were very different. Roald Hoffmann and his wife, Eva, were spending a week at the end of June in Budapest. We taped our conversation during a car ride in the countryside. The transcripts were then sent to Professor Hoffmann for corrections. A few weeks after this conversation, I was visiting Professor Fukui in Kyoto. In this case I had sent my questions to Professor Fukui before my visit and received the prepared answers during our meeting. A few additional questions came up during the actual conversation, to which the answers were delivered while I was still in Kyoto.

The photographs of Professors Fukui and Hoffmann were taken during these meetings.

István Hargittai,
Budapest Technical University,
H-1521 Budapest,
Hungary

ISTVÁN HARGITTAI (IH): Could you please tell us about your schooling and teachers from early ages. How did schools and teachers influence you? How did your interest turn to chemistry?

KENICHI FUKUI (KF): It was in the middle school that I was impressed by the marvellousness of Nature. I was enthusiastic about outdoor activities as a member of a biology-oriented group of pupils, excited by "Souvenirs entomologiques" by Jean Henri Fabre. At the time I was deeply attracted to literary works, particularly of the great Japanese writer Soseki Natsume. These experiences no doubt affected various selections of mine in subsequent life. As a matter of fact, such a Nature-loving tendency was already rooted in the experiences I had in elementary school and in my rather early years spent in my native place. Later, in addition to these, in my high school years I was influenced by Jules-Henri Poincaré through his trilogy of science-philosophy.

The reason for the selection of chemistry is not easy to explain, since chemistry was never my favorite branch in my middle school and high school years. Actually, the fact that my respected Fabre had been a genius in chemistry had captured my heart latently. The difficult point of chemistry for me was that it seemed to require memorization to learn it. I preferred more logical character in chemistry. It was a certain Kyoto University professor who insinuated the hidden logical character implicit in the then prevailing chemistry, and I followed his suggestion after all.

IH: How important is education in determining a future scientist's activities?

KF: Education is a task in which one influences another through the function of both brains, the mechanism of which is still not yet clear. Therefore, what is an ideal education for producing the most active scientists remains an extremely difficult question. Even with the use of auxiliary or subsidiary means in modern education, the direct contact with Nature surrounding the pupil or student seems to me absolutely essential. Of course, in the surrounding Nature the teacher is included as a part of *Nature*. In this context the role of teacher is extraordinarily important. Also, appreciation of all sorts of beauties and goddesses will cultivate pupils' mind to turn to the pursuit of the truth of Nature.

Even in poor schools, such a good teacher will be available and such a teaching attitude will be applicable, to affect gifted children efficiently for their future higher education stages.

IH: What made you prefer theoretical work over experimental?

KF: I originally started as an experimental chemist. I wrote more than 100 papers on experimental chemistry and was awarded a nationwide prize in 1944. Still now, I read papers on experimental studies besides theoretical ones. When I was in charge of supervision in Kyoto University, I assigned experimental work to some of my students as their thesis study. That was because I considered it important even for theoretically oriented students to experience the complexity of chemical phenomena.

It was by chance that I became interested in the chemistry of hydrocarbons. The title of my thesis for graduation from Kyoto University was the chemical reaction of paraffinic hydrocarbons. The work I was engaged in during the first few years after my graduation was on the chemical conversion of olefinic hydrocarbons. And, finally, my first

theoretical paper was on aromatic hydrocarbons. All kinds of hydrocarbons on parade!

It was a very important fact that I had learned quantum mechanics by myself up to then. For me it was natural to attempt to apply quantum mechanics to explain the mode of occurrence of some chemical reactions that had not been sufficiently interpreted theoretically. Aromatic hydrocarbons were just the material.

That was in 1952. After that, my own interest and involvement in theoretical work surpassed that in experimental work. The reason why I had studied quantum mechanics since my entrance into Kyoto University was partly due to my instinctive concern and partly due to the suggestion of a professor.

IH: Who was that professor and how did you choose your subject of research?

KF: The selection of my original research theme was almost determined at the instant of my selection of chemistry. Incited by the suggestion of the professor of applied chemistry, Professor Genitsu Kita, I entered his laboratory. His suggestion was that chemistry, then having a strongly empirical nature, would become a logical science in the future. The theme given to me was the chemistry of hydrocarbons. Rather by instinct, I was strongly attracted by their chemical reactions. At that time their unique chemical behavior was not yet sufficiently interpreted theoretically. Therefore, in my case the original selection of research subject was a combination of chance and intuition. Further developments have been executed in due course.

IH: Was the engineering environment the best one for your studies?

KF: The Japanese university system is rather unusual, and in every large state university the faculty of engineering is larger than the faculty of science. The system of big engineering schools had long been a strange characteristic practice since the Meiji era. In Kyoto University, too, there were six chemistry departments in the engineering faculty while there was only one chemistry department in the science faculty. In my student years, in 1938–41, however, we had the Department of Industrial Chemistry, which was the only department of chemistry in the Faculty of Engineering and larger than the Department of Chemistry in the science faculty. However, we attended the same lectures in fundamental chemistry together with students of pure chemistry. The pure chemistry students had, of course, more chances to listen to lectures of physics or mathematics than the students of applied chemistry. I suppose that such a unique university system is a symbol of a later-developed nation. I had to overcome these disadvantages by self-taught study. The department I chose was industrial chemistry, not chemical engineering. The reason that I chose applied chemistry was very simple. I just followed Professor Kita's suggestion.

Professor Kita was the brother of my father's aunt and had served as guarantor for my father when he was a college student in Tokyo. Professor Kita suggested to my father that his school would be most suitable for me to study in, when my father told the professor that I liked mathematics and physics more than chemistry! Accordingly, the benefit which I might receive by studying practical science was absolutely not in my heart. As a matter of fact, Professor Kita often encouraged his students to study hard fundamental sciences rather than practical sciences.

IH: How did you choose, eventually, your own students?

KF: During the years many students and co-workers joined our group. They were fully familiar with what was going on there. They were all those who wanted to take part in our work. I have regarded their wishes in selecting research themes for them as much as possible.

IH: How do you view the future of computational chemistry?

KF: It cannot be denied that the empirical character of chemistry changed because of recent unexpected progress in instruments for physical measurements and in theoretical chemistry, particularly in quantum-mechanical calculations, using high-speed computers. However, there exist, for instance, in mathematics a number of logical problems that cannot be solved practically on account of the too long machine time required. The complexity of chemistry is such that chemical knowledge expands without cease. The characteristic feature of chemistry lies in its complexity, which surpasses what can be achieved by logical deduction.

IH: Please tell us about your relationship with Roald Hoffmann.

KF: It was in 1964 at a scientific meeting in Florida that I met Roald for the first time. He was then a young researcher. It was four years after his marriage and two years after he got his Ph.D. However, he was well known as a theoretician from his work for his doctoral thesis on a new method of theoretical calculation for molecules. Soon after, the historical papers in collaboration with R. B. Woodward were published. These papers, published in JACS in 1965, which became noted afterwards as the original papers on the so-called Woodward–Hoffmann rules, attracted my attention, since these papers pointed out that

the direction of a chemical reaction was controlled by the phase ("symmetry") of *particular* MOs (molecular orbitals). In 1964, I had learned that the mode of occurrence of a type of chemical reactions was correlated with the phase of particular MOs, the role of which in chemical reactions I had noticed since 1952. In this way, he and I shared our fate to develop our common interest in the same direction. He accepted two postdocs from my laboratory, and they are now active in Japan as excellent professors.

Kenichi Fukui, Kyoto, July, 1994.

In every sense, our mutual relation has continuously been intimate. Even in the past 6 years, he visited our Institute twice and stayed for a while here. All of the members of the Institute enjoyed having Roald visit.

IH: How did the Nobel Prize change your life?

KF: Japan has only very few Nobel prizewinners. As the first awardee in chemistry, I would have become a "darling of the fortune" in journalism. The situation that Yukawa died just before my receiving the prize and Esaki did not live in Japan at that time gave impetus to such circumstances. Needless to say, my academic life would have received disturbance.

However, fortunately or unfortunately, it was the time of my retirement from Kyoto University by the age-limit system applied to every professor without exception. I left the place where I had held an academic position for 39 years. This was in the year after receiving the prize.

A privilege to me was that thoughtful people in Japanese industries built a splendid institute, this Institute for Fundamental Chemistry, for me, and I am able to continue my research in this wonderful site of science.

The big prize did not change my private life very much. Every day I walk from my house to the institute in the same suits and have supper with my wife, sharing a bottle of beer, after coming back home.

IH: What visits to foreign countries and meetings with foreign scientists have influenced you?

KF: I have visited so far more than 25 countries since 1965, attending many scientific meetings and lecturing in many places. For instance, in 1973 I visited 13 states and 18 universities and gave 20 seminars or lectures during my stay in the United States for 55 days. It is almost impossible to specify which was the most influential. All of them were impressive to me, since I had not experienced a long stay abroad during my studies.

IH: How much did you try to communicate with the nonchemist public about your chemistry or about science in general?

KF: I have not been eager to communicate with the nonchemist or nonscientist public about my professional work. This is because my field of chemistry is not suited to amateurs, and because it takes time. However, it is often very difficult to refuse a rush of requests to give talks to the public about chemistry or science in general. So, actually, I am trying to satisfy these requests as much as I can.

IH: What is the perception of fundamental science in Japan? Is it supported adequately?

KF: As is known worldwide, Japan has tried to catch up with western countries since the beginning of this century by importing sciences from them. Now, however, people have learned the importance of promoting fundamental sciences. The materialization of our Institute for Fundamental Chemistry is one such instance. The financial support for fundamental sciences is still much poorer in comparison with that in the United States. However, it is gradually increasing, in contrast with the decreases often seen these last years in some western countries.

IH: How is the image of chemistry in Japan?

KF: Not much different from that in other countries. Chemistry and physics are both becoming not agreeable branches of study for the majority of pupils in high schools as well as in middle schools. Such a trend may come, in my opinion, from human nature. Man instinctively hates the tremendous package of knowledge without limit that is required for study in the course of modern scientific education, which may exceed man's natural capacity. However, in order to cultivate the frontier of chemistry or basic sciences, we need only a fraction of selected students who love science from the bottom of their heart. The general public can utilize the results of science and technology, although they cannot necessarily create them.

IH: How do you suggest that one determine excellence in research?

KF: The evaluation of achievements is always a difficult task in science policy. Truly origi-

nal works are frequently disregarded by the majority of scientists. Obviously, however, hardly understandable works are not always good ones. Citation is no doubt an index that may be used to judge the value of research, but it is apt to be dominated by fashion and current trends, so that the number of citations is strongly dependent upon the field. The judgment of specialists may generally be of significance, while in some cases the intuition or farsightedness of talented nonspecialists may be more reliable than the judgment of the mediocre majority in the field.

The building of the Institute for Fundamental Chemistry in Kyoto. Photograph courtesy of Professor Fukui.

IH: How much disadvantage is there for non-English-speaking scientists to get their papers published in the best journals and to get recognition for their work?

KF: Nowadays the circulation of a journal is one of the decisive concerns for the contributors. Non-English journals, even those written in other European languages, are not favored by the international community of scientists. Therefore, the disadvantage for non-English-speaking scientists like myself is obvious. Additional efforts are usually required to get public recognition for their work. Evidently, this is a big handicap! It should be got over through international intercourses of all sorts.

IH: How do you view the separation of the sciences and the humanities in our times? How can we decrease the gap?

KF: The distances among human, social, and natural sciences are becoming shorter and shorter. This comes from both progress and necessity. The former reason is evident. The progress of physiology and medicine correlates with new methods for psychology and the science of the human mind. The mathematical and computational progress in statistics greatly influences economics, sociology, and politics. Physicochemical sciences promote the progress of archaeology. The examples are numerous.

The latter reason is more important. It comes from the self-accelerating character of science and technology recently becoming appreciable. Science produces new technology, while the results of new technology promote the progress of science. The human native desire intervenes between them. The mutual acceleration of science and technology in this way brought about conveniences and comfort to human life. On the other hand, the uncontrolled development produced serious problems. Nature on the earth and the environment of the earth were seriously changed, and terrible inequality in the distribution of civilization on the earth was caused. In order to affect these circumstances by controlling the perpetual desire of human beings for growth and advance, the cooperation of natural, social, and human sciences is a necessary prerequisite.

IH: How should we be getting prepared for the next century in education?

KF: The generations living in the next century must carry the burden to ameliorate the conditions in which the earth is presently put. For this purpose, they have to make the level of science much higher and apply it to amend the situation, and simultaneously they have to contribute to harmonize the human mind between tolerance and self-restraint. All of these aims can only be expected to be achieved by appropriate education. The importance of education in the future is immense, and the timing is imminent.

In order for the future education not to be hated by subsequent generations, we need some techniques. The package-knowledge type of teaching is evidently inadequate.

IH: Please tell us about your interest and activities outside chemistry.

KF: I was originally an experimental chemist, much interested in organic chemistry, and engaged in some periods in chemical engineering. So, I am not indifferent to industry. To the contrary, I once indulged myself in physics, particularly in theoretical physics in my youth. In my middle school years, biology and literature were my favorite subjects. So my field of interest is rather wide, although my activities outside chemistry were limited.

IH: I understand that you are very much involved with the celebration of the 1200th anniversary of Kyoto.

KF: In July 1984, the Heiankyo 1200th Anniversary Memorial Foundation was established, and the Chairman was Professor Emeritus of Kyoto University Takeo Kuwabara, a noted man of French letters, who was Person of Cultural Merit and Honorary Citizen of Kyoto City. Unfortunately, he suddenly passed away in April 1988. The Governor of Kyoto Prefecture and the Lord Mayor of Kyoto City, who were both Vice-Chairmen of the foundation,

asked me to be the Chairman, and it seemed to me extremely difficult to refuse in the circumstances we then had.

IH: What would be the question you would like to be asked, and, please answer it if possible.

KF: I have already mentioned in the beginning of this conversation that various experiences in my early years affected my life, and how they actually occurred to me. That I was a lover of Nature—forests and rivers, plants, and insects—in my childhood presumably had some connection with my selection of science as my major in my schooling.

Roald Hoffmann, Budapest, June 1994.

That I was fond of reading Soseki's books as a teenager happened to possess a close connection with my selection of a research theme much later. As I mentioned before, the chemistry of hydrocarbons became my speciality after my graduation from university. The then prevailing theories of chemical reactions were not convenient for explaining those of hydrocarbons. Several papers tried, but they did not satisfy my mind's pursuit of a more *natural* theory, since in my memory there remained a story of a dream by Soseki, which had captured my mind. An ancient famous sculptor's art was so free that it seemed as if he only had dug up statues that had originally been buried in timber. Reminded of this story by other scientists' papers which seemed to me not so natural, I decided to search for a more *natural* theory. That was the beginning of my first paper on the quantum mechanical interpretation of chemical reactions of hydrocarbons.

Hoffmann Conversation

ISTVÁN HARGITTAI (IH): First of all, I would like to ask you about your schooling and about your teachers. You write in one of your poems about a boy, presumably yourself, who did not own a book until he was 16.

ROALD HOFFMANN (RH): My schooling was interfered with by the War. First, there were a few months in a Ukrainian school in Zloczow. Then there was the second and third grade in a Catholic school in Krakow in Polish. My fourth grade was taught in Yiddish in a Displaced Persons refugee camp in Austria. Then a little bit in German in Germany, and eventually in the fifth and sixth grade everything was taught in Hebrew in Munich. I learned algebra for the first time in Hebrew. All of this just to show my refugee background, with the mixture of languages that many children in the chaotic postwar period experienced. Then we succeeded in getting to the United States, of course, where all things went well. I attended New York City public schools, first a public school in Brooklyn, then a special science public school called Stuyvesant High School. There was a wonderful concentration of talent in that then all-boys school in New York City. Then I went to college at Columbia. So I grew up in New York City. Eventually I went to graduate school at Harvard.

We were poor; it was not easy for my parents to begin in a new country. So in fact we had no money to buy a book for me until I was 16. I can't remember any particularly inspiring teachers until high school. I remember though that I was not particularly interested in chemistry. At Stuyvesant High School there were advanced courses in every field. They would be called in the United States today advanced placement courses. This was a kind of second course in each subject. I took such courses in biology and physics but not in chemistry. I also took a lot of courses in mathematics. At the end of high school I intended to go into medical research. That would have been a compromise between my parents' desire that I should become a doctor and what I wanted to do, which was some sort of scientific research. I started the university as a premedical student. But that did not last more than a year, and I somehow drifted into chemistry.

I had some unusually good teachers in high school, and they were in mathematics and in biology. At Columbia University the teachers I had in humanities courses were just wonderful. The ones in science courses were okay, but I don't think I hit one that inspired me until the last year in college. I really think that if I had not encountered those teachers in my last year, George Fraenkel and Ralph Halford, I would have gone into the humanities.

The humanities were so seductive, especially the history of art. I had fantastic teachers in Japanese literature, in the history of art, in English literature, poetry, and other literature courses. The world was just opening for me, and those were the most inspiring teachers I had.

IH: What turned you to chemistry?

RH: There were several factors. One was that in my last year in college I took some really good courses in theoretical chemistry. But I think that the main thing was summer research experiences. One was between high school and college, at the then National Bureau of Standards (NBS), then in Washington, D.C. I worked there two summers. The first summer was pretty boring, but it was my first introduction to research. I worked on the thermochemistry of cement with a man named Ed Newman. The very first scientific paper I published appeared in the research journal of NBS, on the heat of formation of hexacalcium aluminoferrite. This is a compound occurring in cement. After that, I knew I did not want to do cement chemistry, but research *was* exciting.

I came back the next summer and had something much more interesting to do. It was the low-temperature pyrolysis of hydrocarbons, low temperature meaning around 500°C. Then the next summer I worked at Brookhaven on some radiochemistry with Gerhard Friedlander and Jim Cummings. We constructed a low-level counting apparatus for carbon-11. That was very exciting. Imagine making a thousand atoms of carbon-11, and measuring quickly their amount while they decayed with a 20-minute half-life!

Although I did not subsequently do any of these kinds of chemistry, they constituted my introduction to real research. They were very important for me, and I still think that for many kids research is the way into science. It does not matter actually what one does in detail, but the social setting of a small group, the closeness to science and scientists, the turning into reality of what is taught in courses, all this is very important.

I could have done other things. However, at that time I thought that I was not good enough for physics, even though I got A's in all my physics courses. I saw kids, my friends, who were better at the subject. Now I know I was wrong and could have done physics just as well. For similar reasons I was pushed away from mathematics. I don't know why, but I was not that interested in biology at that moment in my life.

So you see I came to chemistry rather late and with no strong motivation, except that I got my introduction to research in chemistry. It's true that I had a chemistry kit when I was a kid, but I was not that much in love with the field. I really did not decide to become a chemist until I was 20 years old, or even older.

IH: How would you characterize your relationship with your graduate advisers? What is important for a graduate student?

RH: I worked for my Ph.D. with two people. I started out with Martin Gouterman and finished with William Lipscomb. For both of them I was their first graduate student at Harvard. Originally, I wanted to work for Bill Moffitt, a professor at Harvard, who was the world's leading young theoretician at the time. But he died in the year I came to Cambridge. Martin Gouterman was a postdoc of his who was appointed as an instructor, and then as an assistant professor. Gouterman was a student of Platt's at Chicago and was interested in porphyrin spectra. He is now at the University of Washington, and he continues to be active in spectroscopy and in theory. After about one year of work with Gouterman, I went to Russia for a year, to work with Davydov on exciton theory. Upon my return, I switched to working with Lipscomb. It took only one year of work with Lipscomb to finish my Ph.D. in 1962. Subsequently, during a three-year junior fellowship at Harvard, when I was independent, I developed the collaboration with R.B. Woodward. So I was not a postdoc or a student of Woodward's. There was a different kind of relationship there.

Both Gouterman and Lipscomb were very important to my scientific development, and my interaction with them was really day-to-day. This close contact might be understandable for Gouterman, who was just beginning his academic career. From the moment he started though, he had four graduate students. There was a great demand for doing theory by graduate students at Harvard, and no one on the faculty at the time who wanted to do that. With Lipscomb, who was much further along in his career, there was really also daily interaction.

I remember clearly one important interaction with Gouterman after I had come back from one of Per-Olov Löwdin's great summer schools, where I first learned some group theory. There was someone on the Harvard faculty who was trying to make cubane. I decided I was going to carry out a molecular orbital calculation on cubane. I was very proud of my newfound skills in group theory. So I set up the problem with eight orbitals, one on each carbon, I guess. What I had in mind was a Hückel calculation on eight hydrogen atoms at the corners of the cube, and it was all doable by group theory. I went to Gouterman, showed him the work. He said gently that it was very nice but you have not done cubane, you have done eight hydrogen atoms. And he slowly led me into the complexities of the problem, to setting up the matrix involving all the valence orbitals of cubane. This was essentially a

forerunner of an extended Hückel calculation. He said you must consider 2*s* and 2*p* orbitals on the carbons and the 1*s* on the hydrogens, so that you have a total of 40 basis orbitals for C_8H_8. He said to go ahead and set it up, which I did. Then I did a Hückel-type approximation, and I had all kinds of *s*–*s*, *s*–*p*, and *p*–*p* σ and π interactions. I still have the matrix somewhere in my notebooks, with α's, β's, γ's, δ's, ϵ's, for the various resonance integrals. But I could not go any further, until we had programmed, two to three years later, an extended Hückel program in the Lipscomb group. At the outset I had no idea of taking the β's proportional to the overlap.

Anyway, the interaction with Gouterman was really quite close and with Lipscomb as well. There was also a research group in each case and a lot of learning from other people. I think that from both Lipscomb and Gouterman I learned the importance of interaction with experiment. Lipscomb stressed that a lot.

From Woodward I also learned much. I was at a later stage then, it was now 1964 when I began to work with him. What I learned from Woodward was how to simplify explanations to an absolute essential. It is these simple explanations that make an impact on chemists. You don't have to cloud your explanations in mathematics.

I learned quickly. The first paper I wrote for Lipscomb, or the draft of a paper, was not very good. He revised it extensively. But I learned immediately, and I remember that for the next paper he had only minor changes to make. With Woodward, writing was much more difficult. The language mattered to him, and he rewrote things in excruciating detail. I have a manuscript of the first orbital symmetry paper, with his comments on my draft somewhere. I have always had an easy time writing scientific papers, and that has been important. Since the collaboration with Woodward, my papers have been very pedagogic, taking the time to explain.

There is the question of how to choose research projects. With Woodward, one was looking clearly at important problems (though Woodward saw that more clearly than I). One could argue that part of talent is a kind of differential insight as to what is important and what is not—which anomalies to disregard and which to pay attention to.

Coming back to the teacher–student relationship, I feel that the role of the teacher is to awaken in the mind of the student those capacities which are already in some way there, and that need only that awakening. This idea I think actually goes back to St. Thomas Aquinas. I think it's not a bad summary of what a teacher does. In that sense, I think you need interaction on a continuous basis.

I think students learn in group meetings; and this is a great advantage of the American system. Students have to learn how to discern good science from routine work. In the beginning it's very hard to do that yourself. You need guidance.

Unfortunately, merely studying the chemical literature does not help you. Everything looks great there. You can publish any piece of junk somewhere. I think JACS accepts 60% of all full papers, and that's in one of the best journals. If you go to the next lower quality group of journals, they accept 95% or more. There is just no selectivity in publishing science. The discernment between routine and good occurs at the level of the practicing scientist, who often learns this from group meetings. I learned that from Gouterman, from Lipscomb, from Woodward. It's not important actually what group you're in. What is important is to be in a reasonably international center where there are a lot of seminars, people coming and going, talking about their work. So I think someone in a provincial university in Hungary is in trouble. There the literature might serve as a substitute. To teach the students to go to every seminar in sight is very important.

IH: What was your relationship with Kenichi Fukui?

RH: I met Professor Fukui for the first time during one of his first visits to the United States. I think it was in 1964. At that time I was a Junior Fellow, two years past the Ph.D., and just about to begin the work with Woodward. Fukui came to Harvard to give a talk, and I was pleased to talk to him. I knew him primarily through his work on reactivity indices. Our relationship has always been very good. One reason is that the traditional model of competition in science does not apply to Fukui's and my work. We never actually competed on anything. In a curious and maybe unique way, our work intersected in such ways as to be of benefit to each other, and reinforced the work of each other, without us working directly together.

Fukui came up with his theory of orbital reactivity and the idea of frontier orbitals, the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO). He derived these ideas from perturbation theory. With the formulas he had in place by 1960 (and the most important work was already done in 1955 or around then), he could have solved the problem of the stereospecificity of electrocyclic reactions. But he didn't, because the problem was never posed by experiment. Woodward and I did it first, and we did it essentially with a mix

of extended Hückel calculations and our own "discovery" of the role of frontier orbitals. This was a discovery for ourselves, not a real new finding. We also used perturbation arguments. I knew the Fukui and Dewar papers at the time. Dewar had written that absolutely inscrutable series of four papers or so in JACS in the fifties. It was clear, however, that Dewar was not interested in teaching or explaining specifics; he just liked the generality of his mathematical formulas. Interestingly, Dewar's failure (as a researcher) in these papers was a failure of teaching, I think. So his work had no impact, essentially, on the community he needed to reach.

Fukui was more interested in explaining but was still caught up a little bit with the mathematical formulas and the reactivity indices, very popular then. And he lacked a beautiful experimental case, such as that of the electrocyclic reactions, to demonstrate the power of his approach.

The moment that we did the orbital symmetry work, Fukui could do it. His formalism was certainly up to the task. A reasonable summary of the situation is that our orbital symmetry work with its focusing on HOMO and LUMO reopened interest in the community in Fukui's work. People saw that he had done similar kinds of things, that many reactions could be profitably studied with his formalism.

I don't think Fukui and I competed consciously or unconsciously. Our interaction just worked very well. Subsequently, I had no less than three of Fukui's talented coworkers as my postdocs, Fujimoto, Imamura, and Akagi. I have also visited Kyoto; I was just there last year for a month and a half. I also happen to be interested in Japanese culture from my university days, and I think I also share other interests with Professor Fukui. We get along very well.

IH: How did the Nobel Prize change your life?

RH: The Nobel Prize came when I was fairly young, as these things go, 44. Some consequences were pretty obvious, like many more invitations. In some of those invitations, people were interested in my name rather than in me. This was fairly easy to sort out, but I had to learn how to say no to some things. In general, my life became busier. I had to work a little harder to carve out some time for myself, but I have managed to do that. In many ways it did not change things very much. That's a fortunate thing specific to being in the United States, where there is a substantial number of Nobel prizewinners and where society ignores scientists and their achievements anyway.

For Professor Fukui life was, I suspect, much more difficult, he being the first Japanese Nobel prizewinner in chemistry. He is under much more pressure. No one cares about me (I'm smiling). Even within the scientific community, there is not that much respect or value attached to the Nobel Prize. Just as many negative as positive feelings are engendered. I see occasionally in reviewers' reports, in the darkness, negative feelings come out. People say "I expected a Nobel prizewinner to do better." I have recently (four years ago) lost funding for about half of my research, the work on surfaces, which I think is actually going quite well. My being a Nobel prizewinner has no effect (at least in the United States) on my research support. Linus Pauling has had difficulty getting funding to do chemistry for 30 years. It's a very unforgiving world out there, a very competitive one, in our country.

Being a Nobel prizewinner has helped in no way to get my poems published. My last poetry collection has been making the rounds with publishers for four years, and individual poems go through many rejections before finding a place. What I resent then are assumptions by fellow scientists that things are easier for me. I'd love to show them all those rejection slips.

There is some opportunity to make a fool of yourself. The press is out there, looking for stupid things. So when William Shockley had some weird ideas on race, he found a willing public to listen to that.

There is some barrier that comes between a Nobel prizewinner and students, because students set you up on a pedestal, whereas your colleagues do not, at least not in the United States. This barrier is a negative thing. It stands in the way of informal communication. Fortunately, American students are not too respectful. When I teach first-year chemistry, I know how to overcome that barrier without any trouble. I cannot go to the library to look up a journal article two days before an examination, if I am teaching a first-year course. Immediately I would be surrounded by students asking me about the questions on the examination. I don't think that would happen in Europe.

I think I have had occasionally the opportunity to do things that I could not do before. I was asked to do the *World of Chemistry* films, in part because I was a Nobel prizewinner. What's working here is an image on the part of producers, one that maybe is reflected out there in the world. After making the *World of Chemistry* films, 26 one-half-hour films, we tried to raise money for three prime-time specials about chemistry on

public television (PBS), and we failed. So you see, the name does not mean too much.

Following the Nobel Prize, maybe there were some raised expectations from the scientific community, and maybe some expectations from myself. There has been added pressure, but often from interesting opportunities. But I think the pressure has been generated as much from myself going into different fields as it has by the fact of the Nobel Prize and external demands.

IH: You have used an interesting expression "knowledge is permitted" in one of your poems.

RH: The phrase "knowledge is permitted" comes from a poem I wrote about Sor Juana, a Mexican nun. She had to enter a convent in order to do what she wanted, which was to write poetry. I have always been interested in instances in human history where the spirit and knowledge has come through through periods of oppression or suppression, where it can't be expressed. This is what caught me about Sor Juana's story. Aside from her poetry, she wrote an incredible letter (the *Riguesta*) about the history of women speaking in a church. Her story moved me. In an unpublished lecture about Sor Juana, I remembered something from my vaguely leftist teenage years. It was a German hymn from the middle ages with the line "Die Gedanken sind frei"—"the thoughts are free." I think it was initially a Reformation song, a song of freedom. It was then taken up by the German freethinkers, and I learned it in a leftist context, as a protest song. It was also a leading song of the German opposition to the East German regime in the days of 1987–89, as they struggled toward freedom.

I've always been interested in similar situations. For instance, I've written about the Disputations of Barcelona (again, not yet published). These were staged debates between Christians and Jews. There was one in 1240 (I think) in Paris, in 1274 in Barcelona, and then one around 1290 in Tortola. The Church constructed these forced debates about the merits of the religions, between clerics (who were often converted Jews) and Jewish thinkers. The debate in Barcelona was the most free because the King of Aragon, James I, was powerful with respect to the Church at that point and could guarantee the freedom for the Jews to speak their mind. This debate was another monument to human freedom, at a time when free thought was not possible. There are other examples: K.F. Bonhoeffer's and Otto Hahn's statements at the memorial for Fritz Haber in 1935. I've always been interested in those things.

I think "knowing is permitted" in the context of the poem has several meanings. There is curiosity, a desire to know that cannot be stopped. There must be social responsibility. Should one censor knowledge that leads to evil and destruction, and who should censor it? Should one do research on things that are inimical to the fabric of society? Let me give an example. Should one do research on new weapons or the difference in intelligence between the races? Scientists are doomed to create and must bear responsibility for their creation.

I have been very interested in communist societies, or the thin overlayer which communist societies place on top of the nations. So I have been interested in Russia, China, and Cuba. I spent a year in Moscow in 1960–61. I don't know why I am interested in those things, but I suspect it is mixture of the social justice in socialism and the fight that I have with the suppression of the freedom of expression in these systems.

IH: Did you experience any fallout from the controversy about the theory of resonance while you were in Moscow?

RH: That also has interested me a great deal. The proceedings of the 1951 conference constitute a beautiful case study of survival in the Russian scientific climate of that time. This is the Lysenko period, the last days of Stalin. Given Lysenko's success in questioning Russian scientific authority, in every field, opportunists, politicians, and publicists outside of science created Lysenko type problems. In chemistry we had the controversy about resonance theory, condemned for being idealist. Really, it was opportunism and politics at work. In this particular case, what was under the table, and not obviously discussed, was that the opportunist attack was not only on the theory of resonance, but it was also an attack on the leadership of Soviet chemistry, on Nesmeyanov, who was then the head of the Academy of Sciences. The attack was led by a scientifically illiterate chemistry professor at the Moscow Military Academy, Chelintsev.

How this could have happened, and how Soviet chemistry was saved, and how Nesmeyanov kept his job, is a fascinating story. Some sacrificial lambs were offered in the persons of Syrkin and Dyatkina, and Vol'kenstein in Leningrad. Syrkin and Dyatkina lost their jobs, which was terribly sad. They still remained influential through their students.

Another reason that the proceedings of the resonance theory conference are interesting is that there are occasional hints, in them, in the printed text, of opposition. There are brave anonymous questions from the floor. It's also very interesting to see who gained ascendance in

that period through the stance they took in that controversy. Some people, in fact, made their name through this, by supporting the wrong, irrational side. People such as Tatevskii in Moscow University, and the physical organic chemist Reutov. I have not forgotten them and Russian chemists have not forgotten them either.

Many of the people involved were forced to write abjurations of what they did, in various books. There is a sad episode around the time I was there. Pauling came to Russia. Pauling presented real problems to the Russians, because for political reasons he was a friend, an advocate for peace and disarmament, but here he was suddenly the subject of this controversy and on the "wrong" side. Finally, they invited him for propaganda's sake, and Pauling came. He quite insensitively spent most of his time in Russia criticizing those books by Vol'kenstein and others. Everyone knew why they had written those books, to save their positions. But Pauling just was not sensitive enough to this, and whereas everyone else wanted to forget about those books, eight years later, after the controversy, Pauling criticized those books. But that's the way he is.

I remember that during my stay in Moscow the classic book *Molecular Vibrations* by Wilson, Decius, and Cross came out in Russian translation. The preface to it, I think, was written by Tatevskii, who somehow managed to drag in the theory of resonance. It was startling to me to see an opportunist keeping things alive nine years after the controversy.

There is no question in my mind that the resonance theory controversy kept young people from theoretical chemistry in Russia for a good number of years, at least for ten years. A country that was in good shape in theoretical chemistry was set back. The scientists suffered, which in itself was a great loss; I have already mentioned Syrkin and Dyatkina, who both were very, very talented. Young Russians, for a long time after that, did not feel comfortable with theoretical chemistry. People negotiate their progress in those societies within the context of what is allowed and what is not. Sometimes this is done in subtle ways. A young Russian, talented, chemist or physicist, thinking about what he's going to do in his career, trying to decide between theoretical chemistry and something else, would in various unwritten, unspoken ways get the signal that theoretical chemistry was somehow a little dangerous. Even if that young person were doing molecular orbital theory, which was not the subject of the criticism directly, it was probably better to go away and do something safer, like solid state physics. I think that through that mechanism many talented people were lost to theoretical chemistry in Russia.

IH: How about writing poetry? Do you need suffering for writing good poetry?

RH: I think this is a piece of a popular myth, that suffering helps creativity. There is a poem about this subject in my first book, entitled "Admission Price." It is a romantic fallacy that to be creative in art you have to be at the edge of madness. I don't think you have to suffer to write good poetry. Nevertheless, human life is full of suffering, at every level.

Poetry has been important to me. At the beginning I was just reading, I did not start writing until I was about 40 years old. Right now, the poetry is a little slow, and the essays and books are going much better. I just finished a book called *The Same and Not the Same*, which will be out next year. It is intended for the general public and certainly is about chemistry. I sort of like things falling into place; I don't start out writing a book with a theme, but I let the theme come together from smaller pieces of writing. Perhaps this comes out of my poetry.

IH: How does your language interact with your writing, and how did you change from one language to another?

RH: My first language was Polish. Ukrainian and Yiddish were also around, and I knew them early on. Then came German, followed by Hebrew. Children learn quickly and forget quickly. By the time I came at age 11 to the United States, German was my dominant language. Then English took over. I was not very nice to my parents; I made them speak English to me.

Four languages were spoken interchangeably at home: Polish, Yiddish, English, and German. Subsequently, I learned two other languages well, Russian and Swedish, for one reason or another, and another language, French, not so well because I studied it only at school. English is, however, the only language in which I can write; it *is* my native language. Native speakers may detect a slight accent in it, and I have just a few small problems in the writing occasionally, such as confusing "like" and "as" and "that" and "which." Occasionally, my constructions are a little funny, but English is my language and I love it.

I think more important to writing may be being an outsider. Knowing several languages puts you a little outside the one language you have been thinking in. You ponder of things more than the native speakers.

Being an outsider comes from being an immigrant in a

society. And Jews have been outsiders in other ways. I have also switched subfields of chemistry; I felt like an outsider when I started in organic and in inorganic chemistry. I sort of like that feeling, for you get a different perspective. Coming from the outside, at first it's a little dangerous and difficult but I like the feeling of penetrating the walls built of jargon and custom around a field.

IH: Please tell us something about the TV series you participated in.

RH: Its title is *World of Chemistry*, and it is a series of 26 half-hour TV programs. It's now a few years since we made it. The programs have had a reasonable reception in the United States. Their main use has been at the high school level, although originally the series was designed at the junior college level. The telecourse is best used in conjunction with a good teacher talking before and after the films. On television in the United States it's on at various hours, whenever the cable channels put it on. The films have been very successful in Israel and Sweden; they are available for international distribution elsewhere, at some cost. I don't get anything out of the sales. I was paid a fee, but I used the fee essentially to replace my salary from Cornell for the year when this was being done, so I could take a leave. I am happy that we made the series. I was one cog in the wheel; we were six academic people involved, and the others in fact worked harder than I did on this. Television is one set of compromises with the material after another. But what a way to reach people!

We tried subsequently to make a three-hour PBS series, in which I was to play a more leading role as a scientific director, and I wrote the scripts for it. But in the end we were not able to raise enough money for the project (we need $1.35 million) in spite of tremendous help from the American Chemical Society. We were given good support by foundations but not by the chemical industry. I think industry is rather short-sighted in these things, and not only American industry, for we tried Japanese and German companies as well. We had to give that up. This is one of my failures.

IH: How about *Chemistry Imagined?*

RH: This book and art exhibit came out of a meeting with a talented artist, Vivian Torrence. I thought that her impressions of chemistry were intriguing and would help form an image of chemistry for the intelligent lay public. Vivian's work has a kind of intellectual feeling to it, and a deep understanding of art and science. I have always been interested in interaction with artists. I also thought of the book in terms of an audience of people who are around chemists. Something that a chemist would give to a nonchemist friend. Not to teach about chemistry directly, but to tell people of the spirit of what chemists do. I also thought of *Chemistry Imagined* as a work of art and literature. It has a novel construction, a collage of essays, collages and poems. I also thought about its similarity to emblem books of the Renaissance, these marvellous products of the sixteenth century where there was a motto, a picture, often enigmatic, and some text connected to the picture. As our book evolved, I saw in it also something about shaping interactions between art and science, about moving across borders.

I like to think that everything I do about chemistry shows chemistry as an integrated part of our existence, of the economy, social structures, art, of the intellect, creativity as well as utility.

IH: How much does outside support determine what you do?

RH: This depends. The poetry is a small personal enterprise. I could do it without any support, and I do do it so. Making the TV series would have been just impossible, as it cost $2.3 million. *Chemistry Imagined* is an in-between thing. Probably we would have done it without the $ 90,000 grant from the National Science Foundation that helped Vivian to live while she was working on the collages. The new book I am doing for Columbia University Press I would have done anyway.

I don't actually expect society to support my interdisciplinary activities very much. Of course, I get a bit unhappy when I reach out for some support and it is denied. There is a book I'm writing with Shira Leibowitz, on science and religion, for which we have failed to get support (despite trying) from the National Endowment for the Humanities and from the National Science Foundation. We have received an advance from the publisher, but that's not enough to support Shira and me while we are doing it. So we'll do that project on our own.

Ideally, it would be nice to have a Maecenas who would give me $100,000 a year to do what I want to do. I really don't expect that. My greatest disappointment is not that *society* does not support these things, but that *fellow scientists* don't. I am unhappy when scientists don't seem to be interested in a project as unique and original as *Chemistry Imagined*. We were unable to have it reviewed in *Nature* or in *New Scientist* or in *Science* or in *Scientific American*. This is a failure of the individual chemists (editors) who could have got-

ten us those reviews. But then I think of the lukewarm reception in the chemistry community to absolute classics, such as Primo Levi's books, when they first appeared.

My poetry books had good sales, the first one (1987) 1300 and the second one (1990) about 900. That's actually very good for poetry books. But I know that there are 150,000 members of the American Chemical Society out there, that $14.95 is not much money for a book, and I was hoping that a few more would buy them. There are not that many poetry books written by scientists.

IH: How about education as we enter the twenty-first century?

RH: Education is a conservative enterprise, and it does not change very quickly. I think the shift in chemistry education has to come from the recognition of the fact that 99.9% of the population are not going to be chemists. Recognizing this is especially difficult for the Europeans, as chemists there usually teach future chemists, whereas in American universities we teach the masses. The perception of the necessity is clear in the United States and will become clearer as government decreases funding or imposes utility as a criterion for support. We have to educate people outside of chemistry, who become our leaders.

Courses will have to be constructed for the general public. To be responsible citizens, people have to make decisions which are, in part, based on technological and scientific issues. Those decisions should not be left to experts. We know very well that experts can be marshaled on any side of an issue that you want. You want to site a dam or an incineration plant and you can get experts who tell you that there is no danger at all and you can get experts who tell you that there is going to be damage from it. There is a role for experts, but the public has to decide by themselves. For this, they need to know a little chemistry.

IH: Gay Lussac said something about 150 years ago about the day when we shall be able to calculate everything in chemistry that we can only measure today. Then I heard people saying that experiments should be replaced by calculations. How do you view this?

RH: Of course, I don't agree. I think chemistry has an infinity of ways of renewing itself. Our wonderful science is the making of molecules and their transformations. I take much heart from physics, which is a more theoretical science than chemistry. Has it been reduced to calculations? While accepting a theoretical ideology, physics remains an experimental science.

I think there are many things that can be calculated, and it is interesting to see how molecular modeling has indeed entered the everyday life of the organic chemist. But I think that chemistry will not be replaced by calculation. Maybe that's in some sense a hope that comes out of being older, but I don't think so.

In fact, I take heart in a perverse way from the fact that the more people calculate, the less they understand. To understand means to me to sense trends and to sense relationships, to know the physical mechanisms that make an observable. To understand means to make an order-of-magnitude estimate, to talk qualitatively about the next member of the series. Then to use to the computer to get the quantitative numbers.

Let's say that the dipole moment of water is calculated. Then you ask about the dipole moment of methanol or ethanol, and the computational chemist says, wait a minute, I'll have to go back to my computer and calculate it. That's far away from understanding to me.

IH: How to assess excellence in research?

RH: There are no good ways, although there are many criteria that are partially valid. Citation frequency and impact factors have something to do with it, but sometimes they have very little to do with it. Short-term citation frequency may not be relevant. Once I was asked to comment by Eugene Garfield on the top ten chemistry articles in 1991 or 1992. They produced for me a list, based on recent citation frequency, and *every one* of the top ten was on fullerene chemistry. What they wanted was to spot *the* hot new field. What they spotted was *a* hot new field plus fashion. Twenty years later, you may get a different picture. You probably will be better off in establishing excellence by polling a group of people, including experts and ordinary chemists, workers in the gardens of chemistry. In such an evaluation, of course, you must eliminate self-citation and citations by the same school. In any case, human beings and subjective judgments must be involved in the evaluation.

IH: Finally, what question would you have asked of Roald Hoffmann?

RH: I'm glad you didn't ask the question of what development I foresee in chemistry in 20 years or something like that. That would have been a terrible question. I just don't like to prognosticate. I think chemistry evolves nicely in its own random, chaotic fashion. The new chemistry, certain to be exciting, is also certain to escape my limited foresight.

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Dr. Alfred Bader
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Milwaukee, Wisconsin 53202

Dear Alfred: November 30, 1995

Thank you very much for the opportunity to visit with you and Isabel and, on top of everything, for your thanking me and Magdi for our visit. We both enjoyed it a great deal. Special thanks for the agent's name and address. I may be writing him soon and in that case I would be sending you a copy of my letter.

I know that you are now away until December 24 but I am sending you this letter anyway because I would like to keep you informed and there are several things in motion.

Buchan/Three Boards
I am enclosing a copy of my letter and the suggested revised version. I like to think that my version makes the story even more focused.

Bader/Chemophobia
I am planning to have it in the magazine.

Although these two items are sufficiently different, it may be better to run them in separate issues. A brief review of your book will be going into one of the next issues, most probably the April issue which is the next available. It is the easiest to have because it needs the least space. Also, the book review may be in the same issue as one of the other two longer pieces. I have doubts though about my own interview because there is quite a bit of overlap between the interview on the one hand and the Buchan paper and the book review on the other.

In any case, the interview went very well, although I have not yet transcribed it, it will be excellent material. If it is not sufficiently different from the other "Bader-related" pieces, to be published in the magazine, I'd still be using it in the book I am planning to make from the interviews. Otherwise, I think I should be giving preference to the pieces authored by others rather than by myself.

Many thanks for getting me onto the Aldrichimica Acta mailing list; I already received an issue.

I am very happy about the relationship we seem to be building up, and I would not like to spoil it in any way. However, I would not be entirely honest if I would shy away from the following question. You seem to be interested in good causes to support. I would be happy to make suggestions if you had any interest, for example in a Bader prize for students at our School or other things. I'll also understand it if you don't want to extend such activities in new directions or in this direction. Our University has an excellent Foundation which provides the most suitable means for administering such actions.

In this connection, again, for sake of absolute honesty, it has bothered me what you mentioned about the low level of research support of British schools and in particular Sussex. Whatever support they can get I am happy about. Nonetheless I wish we had their problems and their difficulties. I understand your special attachment to British and Czech and Canadian causes and I admire you for that and I am happy for my colleagues there. It's only that when I am comparing our conditions with those of my good friend Harry Kroto, for example, I find it hard to stay nothing when I hear about their complaints.

With kind regards,

Yours sincerely,

and I know how impertinent I am

The
Chemical Intelligencer

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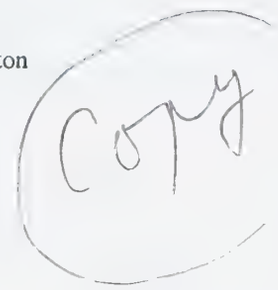

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Dear Dr. Buchan:

November 28, 1995

It was very good to talk with you on the phone during my visit in Milwaukee. I have read your manuscript so many times that I decided to make an attempt to reduce it and I am enclosing the result. Please, consider it for what it is, a suggestion. For the starting pages and towards the end we could probably use a few more subtitles.

The original manuscript was too long for our magazine. On the other hand, I understand your desire to be as complete as possible. In this there is some conflict, of course, since our magazine is informative and entertaining but cannot be the forum of documents of almost legal completeness. We simply don't have the space for it and also, it is not too interesting to a broad circle of readers. I believe that the way I reduced the material retains a fairness of the presentation and can maintain the interest of most readers even though they are not involved in this argument. However, I repeat and stress that this is merely a suggestion. In any case, you will be able to see the faults of the original text if I have misunderstood many things and my faults too but, as I'd said, I truly read the whole thing several times. In many cases, but by far not in all, I felt I was eliminating parts that were repeated elsewhere in the text.

In fact I would not mind to reduce the text further by about fifteen per cent so that the article would not be taking up more than four printed pages in the magazine. However, this is not a requirement merely a wish. It may also be that you would like to do the reduction in a different way, after all, this is your article. In fact, I would also like to get a photo of yourself and a few lines of a biosketch about your background and interests. These would be given at the end of your article. Of course, this is optional but would be of interest. We do this in most cases, and yours would even be more intriguing because you are, obviously not a chemist. Thanks.

I am sending a copy of this to Dr. Bader asking him sort of review this version, but asking him to do so only if you like the changes I had introduced. I was trying to delete parts of your text and introduced actual changes sparingly. So almost all if not all the sentences are still yours.

Two questions. I have somewhat changed the Emerson quotation, please, check it. The way you used it gave me the impression as if the text had been dictated but not checked afterwards. I may be wrong completely.

The other question is whether the Cori parents shared the Nobel prize and in what field. From the formulation of your sentence it is not clear to me whether they got the same prize shared or they got separate prizes. It may also be my insufficient English.

I'll be looking forward to hearing from you,

buchan.doc, word count 4,574

Three Boards and "A Bet Against THE Company"

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The Russell Hotel in the Bloomsbury district of London was an attractive but unusual location for the three businessmen, two from Milwaukee and one from St. Louis, to hold a meeting Wednesday, on November 20, 1991. They were the three most senior officers of the Sigma-Aldrich Company and one, the eldest, was about to be terminated; not in the Mafia sense but the corporate sense. Dr. Alfred Bader was the only one of the three who did not know the real purpose of the meeting. The other two, Dr. Tom Cori, Chairman, President and CEO, and Dr. David Harvey; Chief Operating officer knew, but they also knew that it wasn't going to be a pleasant task. Was there some solace from knowing that they were simply carrying out the wishes of the Board?

The previous Friday, November 15th, Dr. Cori had phoned Dr. Bader, who was visiting the chemistry department of his alma mater, Queen's University. When the call arrived Bader had just delivered a lecture on "Challenges at Sigma-Aldrich", which was a personal history of the company he had helped to found. Although his voice was quiet, each phrase painted a vivid picture of the challenges, the set-backs, the victories. There was still a trace of a German accent. The structure of his talk reflected the precise, orderly mind of the scientist but the content also reflected a literate mind which admired the power of the English language to captivate and excite. As an undergraduate he had been impressed by the animated prose of Thomas Babbington Macaulay, the 19th century English historian and essayist. Despite being in Canada for only a few years, despite his German accent, he won the Dominion of Canada University debating championship.

As he reviewed the early years of the company, he amused his audience with the story of the very large chemical company (Kodak) which announced that it no longer wanted to be bothered directly with small orders for specialty chemicals. This declaration had inspired him to take an ad in the chemical journals inviting his customers "please bother us".

Bader delivered a second lecture that morning in the art history department, "Adventures of a Chemist Collector". In the evening, he gave yet a third lecture on Jan Lievens, a Dutch painter of the "grand epic manner". His final lecture on "The Bible through Dutch Eyes" was scheduled for Saturday afternoon in the art centre. The diversity of the subject matter of these lectures captured the essence of the interests and the career of the sixty-seven year old Bader. Art, the Bible and Chemistry (and his Company) were often referred to as the ABC of his life. A life which had taken a significant turn on November 15, 1941 when he had first enrolled in Queen's University as a teen-aged Jewish refugee. The purpose of the special reception by the University and the lectures was to celebrate the 50th anniversary of this event.

At the Russel Hotel meeting, in London, Cori jumped right to the point and told Bader that there was no room on the Board for anyone who would "bet against the company"; and his selling of stock options had been just that. In light of this action the Board was unanimous in its request for his resignation.

Bader was stunned. He was being accused of betting against the company. HIS company? Because he sold 100 options on some of his Sigma-Aldrich stock? If selling 100 options (for 10,000 shares) was a bet against the company what was the retention of the other 3.7 million shares that he owned? Although his shares represented only some 7% of the outstanding shares in the company he was still its largest private shareholder. The sale of the call-options had simply been part of his planned gift of 10,000 shares to Queen's.

Bader was not going to let his career come to such an ignominious end. He phoned and/or wrote to each of the outside directors arguing his case. Although the reactions varied the message was the same, "He should not have bet against the company."

On December 30 a notice went up on the Aldrich bulletin board, announcing the end of Bader's consulting contract and wishing him well in his retirement.

Bader still would not give up. He and Marvin Klitsner were still directors until the annual meeting of the Board in May. Marvin was Bader's closest friend and business advisor and had been a director of Sigma-Aldrich since the merger and prior to that a director of Aldrich Chemicals from its early years.

Bader and Klitsner, the last of the Alrich board members, appeared before the nominating committee at its February meeting and presented their case as strongly as they could, vigorously denying they had bet against the company. They emphasized that the options they had sold were "covered" call options, which meant the shares were committed at the time of the sale. Technically they had not reported the sale of the options as promptly as they should have. But it was a new regulation and both had reported their sales as soon as they had become aware of the need to do so. The company's own meager memo on the subject had made no mention of options trading. Had it done so they undoubtedly would have met that deadline requirement as well.

However, the Board had not wavered from its position taken last November and Bader had full measure of the extent to which he had grown out of touch with his fellow board members.

Indeed the Sigma-Aldrich Board of the 1990s was very different from the Board of the 1980s and a world apart from the Aldrich Board of the 1960s and 1970s. The evolution of the board was a reflection of the evolution of the company and a classic example of the separation of ownership and control and, for the original owner, it held tragic consequences.

The Board of the 60's was Bader's Board. Following the merger of Aldrich with Sigma-International in 1974 and for the next decade the board was a Compromise Board. During the last half of the eighties a new Modern Board emerged; one however, which also reflected the preferences and comfort factor of the President and Chief Executive Officer of Sigma-Aldrich.

To understand the different character of these three boards we have to understand the history of the company, and for this we have to understand a major part of the life of Alfred Bader, for, as Emerson once observed, "an organization is the lengthened shadow of one man".

Queen's University was already two months into its fall term of 1941 when Alfred Bader enrolled in the Engineering Chemistry program. He had a lot of catching up to do, but he did and then went on to fulfill the requirements for both the B. Sc. and M. Sc. degrees. He continued further and completed his doctoral studies at Harvard in 1949 and then accepted a job with Pittsburgh Plate and Glass (PPG) in its paint research laboratory in Milwaukee.

While working in the Harvard lab, Bader had become frustrated waiting for delivery of a basic chemical needed to carry out his experiments. The specialty chemical was offered by only one large chemical company, Eastman Kodak and it had more important products on its priority list. In response to a follow-up memo from Bader, Eastman Kodak sent him a postcard telling him they would send the chemical as soon as it became available but, in the meantime, would he stop adding to their paper work.

Shortly after joining PPG's laboratory, Bader recommended that a small division within PPG be set up to make and sell specialty chemicals. The proposal was turned down; why even try to compete with Eastman Kodak? However, there would be no strong objection if he started his own enterprise on his own time, provided it did not interfere with his work with PPG. Bader the chemist, became Bader the entrepreneur, the one who saw a commonly experienced frustration as a business opportunity.

First year sales were only $1,705, but rose to $5,400 in the second, and in the third year sales almost tripled to $15,000. When PPG decided, in 1954, to move its Milwaukee laboratory to Springdale, near Pittsburgh, Bader elected to stay in Milwaukee and to devote full time to the fledgling enterprise.

The company's target market was clearly defined from the very beginning; chemists in research labs who needed specialty chemicals to carry out their research. The products would usually play a small, but very vital part, in the activities of the laboratory. Although the chemical might be expensive on a unit basis, the number of units required was small, and the actual cost was insignificant relative to the overall cost of the experiment. However, the product had to be of reliable quality, not necessarily perfect, but good, and it had to be available quickly.

To buy the necessary products Bader had to travel outside Milwaukee. The potential suppliers of the products were any laboratory in the world and some of the best laboratories were located in Germany, England, and Switzerland. Bader was obviously fluent in German and English and spoke passable French. He began canvassing laboratories throughout the United States and Europe. As a research chemist he could talk their language, recognize who were the top producers, what were their needs, what were their problems and as a businessman how could he help them in their work?

It was a relatively easy matter to identify the commercial and academic research laboratories and to communicate with them. A simple catalog would be sufficient to identify Aldrich's product line. Indeed, Aldrich's first catalog was one page, with one product, a product he had learned to make in the laboratory of Prof. A. F. McKay while working on his M. Sc. degree at Queen's. By 1965, the company cataloged over 9,000 different chemicals, with its best selling chemical accounting for no more than 2% of its total sales, and no other chemical accounting for as much as 1% of its total sales. The Company's customers included many substantial industries throughout the world, the federal government, universities and laboratories doing medical research. The federal government's laboratories accounted for less than 10% of the company's sales and no private concern accounted for as much as 5% of sales. Regionally, 80% of the sales were in the United states, 10% west of the Rockies, and 45% each in the Midwest and the East. Foreign sales were distributed across 20 countries usually through foreign agents.

The diversity of the company's product line and customer base provided a stable foundation for its explosive growth. Marketing its products through the catalog was relatively easy, effective and, best of all, no expensive sales force was required.

By 1965 the company manufactured approximately 15% of its sales, purchased approximately 10% from a German affiliate (EGA), and the rest from many different sources none of which supplied more than 10%. The company's strategy was to manufacture only those products that it could not buy advantageously from other sources. Even when it did initiate new chemicals in its own facilities it would farm these out to other producers whenever it was worthier to do so. No company could afford to build production facilities that would ensure adequate supplies of the thousands of rare chemicals used sparingly.

The Art of the Deal

Bader the owner-manager, personally visited laboratories throughout the world to locate reliable sources of the specialty chemicals that were the backbone of his product line. He selected the chemists who staffed the company's laboratories and kept close contact with all the employees in the office and those who handled the shipping and receiving.

To ensure product quality, to develop new products, and continue the dialogue with his research customers he created an organization in which leading scientists played a key role. By 1965 there were 125 people in the organization of whom 34 were graduate chemists with no fewer than 9 holding Ph. D. degrees in chemistry. There were an equal number of office employees and the rest were directly involved in the shipping and receiving of orders and plant maintenance. All but nine employees were located in Milwaukee.

For all intents and purposes the Aldrich strategy was neither to discover nor produce new specialty chemicals, although it did both. Its strategy was much simpler; to purchase and distribute specialty and rare chemicals to people who needed them.

The Success of Aldrich

By 1965, a decade from the time Bader decided to devote full time to his specialty chemical company, revenues had increased from $34,000 to over $2,000,000. Profits were increasing rapidly as well, reaching almost $200,000 in 1965, and profit margins, were some 20% before taxes. But the company was just in the lift-off stage. By 1970 sales had tripled to almost $6,000,000 and profits (before taxes) increased almost fourfold to $843,495. And it continued, by 1974 (the last year before the merger) sales had almost doubled again to over $11,000,000 and profits had more than doubled to almost $3,000,000.

The Bader Board of the 1960s

The Board of Directors which oversaw this evolution was relatively small and made up mainly of insiders. Between 1961 and 1974 there were eleven directors who served on Aldrich's board at one time or another. The only two who served throughout the period were Alfred Bader and Marvin Klitsner. The other insiders through 1967 were: Helen Bader, Alfred's first wife, who was also the company's Treasurer, John Biel a ~~medical~~ chemist, VP and Director of Research, and William Buth, also a chemist, VP and Director of Operations.

By 1970 the Board was very much less an "inside" Board but the "outsiders" had very strong links with the company in a direct business sense.

In 1971/72, one of the last appointments before the merger was Dr. H. C. Brown of Purdue who had developed a process that permitted the production of hundreds of compounds by hydroboration. Aldrich bought exclusive right to Brown's patents and set up a wholly owned subsidiary (Aldrich-Boranes Inc.) to produce the products.

Although Bader was the art collector it was the other inside directors who suggested putting the old master paintings on the cover of the company's catalog. The paintings, all from Bader's personal collection, soon became an Aldrich hallmark.

The Merger

By the early seventies Bader began to see the advantages of a still bigger operation, especially from the financial market's perspective. Taking the company public in 1965 had not generated the interest among the investing community that he had hoped for. Another way of achieving his company to expand could be through a merger. One company that had caught his eye was Sigma-International, almost a clone of Aldrich except that its field was biochemistry, and it dominated the biochemical laboratory sector.

The two companies merged in 1975 forming Sigma-Aldrich. Combined net sales in 1975 were $43 million, and profits, before taxes, $11 million.

The Compromise Board, Sigma-Aldrich 1975-85

Immediately following the merger, the Board consisted of eight directors, 4 each from Sigma and Aldrich. The Aldrich directors, chosen by Bader were A. Bader, who became President of Sigma-Aldrich, H.C. Brown, R. Emanuel, and M. Klitsner. Brown's appointment to the Board was not renewed in 1978. The following year he received the Nobel prize in chemistry.

The directors appointed by Sigma were D. Broida, A. Fischer, J. W. Sandweiss, and S. J. Weinberg. Broida, Bader's counterpart at Sigma, became Chairman of Sigma-Aldrich. A. Fischer, who might also be considered a founder owner of Sigma, had hired Broida (in 1936) into the small consulting firm, which he and his brother had started in 1934. Sigma was started in the early 1950's under the umbrella of the consulting firm, but was created almost entirely through the initiative of Dan Broida.

The Sigma-Aldrich Board was increased by two in 1977 and that was when Dr. C. T. Cori joined. Cori, who had been a Vice-president of Sigma-Aldrich since the merger, was promoted to President of Sigma in July of 1976 (succeeding D. Broida). Cori's rise through the ranks was quite exceptional, having just joined Sigma in 1970 as a production chemist, fresh out of the University of Washington (Missouri) with a Ph. D. in biochemistry. His parents, Carl and Gerti were exceptional scientists who had both won the Nobel prize in 1947 for their work on carbohydrate metabolism and enzymes.

In 1983 Cori became the CEO while Bader retained his position as Chairman of the Board. Throughout, Bader focused most of his attention to the vital liaison work with customers and suppliers around the world the primary difference now was that any new leads on biochemical products were turned over to Sigma. The overall management of Sigma-Aldrich was left in the hands of the aggressive CEO.

The Modern Board

In 1985, a re-organization plan was prepared by Cori which envisaged a larger Board and increased representation by "outside" directors. Only Bader and Klitsner remained from the Aldrich Board. One outside director described his views on Boards in general:

"... How people got on the board, and what they think they were put on the board for is important. And getting the board to come together and be willing to have a few good fights, on an equal basis, and get rid of egos. Getting rid of egos is a very important part of getting value out of the board. It's not easy to get a bunch of high-powered guys - who are, in their own right, successful and important to some extent - to be prepared to look at the issues of another entity without getting their egos in the act. It can screw things up considerably when they do."

A Change in the Chairmanship

Bader learned who controlled the Board in the spring of 1991 when he was forced to resign as Chairman. He was given the title of chairman emeritus and remained a director. In this capacity he continued his duties, now almost exclusively devoted to external liaison activities with customers and suppliers. Arguably he was the most widely recognized chemical executive in the academic research world (he held six honorary degrees from universities in the United States, Canada,and Britain).

The view implanted in the minds of some Board members was that Bader was a charming but somewhat primordial gentleman more at home with professors than real businessmen. How would an objective, independent director determine the real value of the man? One of the hottest topics around Board Rooms these days is what is referred to as the "dual problem". Should the CEO of an enterprise also hold the post of Chairman of the Board? There is an increasing movement among Corporate America towards splitting the two positions and towards reserving the Chairman's position for an outside director only.

In May, 1991 Dr. Cori became the Chairman of the company as well as its President and CEO. He occupied all the key positions.

Six months later on the evening of November 11, at the reception for the Sigma-Aldrich directors, Marvin Klitsner informed Tom Cori that he had been selling options on his holdings of Sigma-Aldrich stock. He had just learned that there were new SEC regulations that required directors and officers to report such sales and he had just sent in the necessary forms to the SEC. Cori's concern was to ensure that any short term profits be returned to the company in compliance with the law.

Following the board meeting the next day Cori and Bader had gotten together to draft out, in rough terms, Bader's assignment for the next year. Cori had made it clear that Bader would not receive any salary but if he wished to continue his liaison work, his expenses, office and secretarial requirements would be covered.

On November 13th, Cori learned that not only had Marvin Klitsner been selling stock options but so had Alfred Bader. He phoned Bader in Milwaukee and angrily charged him and Marvin with selling options "in concert." Bader had sold, on one occasion, some stock options but it was not in concert with Marvin, rather it was part of his planned gift of 10,000 shares to his alma mater, Queen's University. He had just learned that such sales needed to be reported to the SEC and the forms were already signed and a copy was on its way to Cori in St. Louis. Cori advised Bader that he was going to leave the matter in the hands of the company's lawyers.

When Bader sold the options on August 15, 1991, Sigma-Aldrich shares were trading at $43. He got $2 5/8 for each of the 10,000 shares ($26,250) covered under the option. The purchaser of the options received the right to buy the shares at the strike price of $45 any time up to the options' expire date on January 17, 1992. Bader planned to give the proceeds from

the options plus the covering 10,000 shares as part of his pledged gift to the University and it would be ahead by the $26,250. Only if share prices rose above $47 5/8 would the University be worse off. In fact the price of the shares rose to $52 and Bader sent the University another check for $50,000 to cover brokerage fees and to ensure that his $2,000,000 pledge was reached. He had been for some time one of the University's more generous benefactors. In 1990, for example, his donations exceeded $750,000; in the Spring of 1991 he had pledged more than $2,000,000 towards a chair in chemistry, a chair in art history and, the art gallery.

The generosity of Bader and his family to his Universities and the greater Milwaukee community is widely known and so it is unlikely that any informed observer would label his sale of the stock option as an "ex-post facto" attempt to gain sympathy for certain sly stock activities. But why might the reasonable, rational observer consider the sale of stock options, by an insider, to be a bet against the company? What is the origin and the validity of the argument underlying the phrase, bet against the company? The new regulations issued by the SEC in 1991 were designed to bring the trading of options under the same regulations which governed insider trading of stocks. Any "short swing profits" were to be subject to disgorgement by the company; i.e., any officer or director, considered an insider, would have to return to the company any profits realized within 6 months of the transaction. The intent, stemming from the abuses in the market during the 1920's and 1930's, was to protect the general investor from those who might have "inside information" not generally available to the public. There was no need to prove that such information existed or that the insider knew of such information. All such profits were to be returned to the company. The act was considered blunt but effective, even if somewhat crude and simplistic. It did not prohibit the trading of stocks or stock options but simply eliminated any short swing profits by insiders and hence removed any incentive to engage in such activities. Before the 1991 regulations it was not clear whether the old regulations even applied to option trading. Generally, trading in options, by insiders, is frowned upon because it might be construed as a "bet against" the company. When a person sells an option he is, in a sense, gambling that the price will not rise above the strike price ($45 in this case) during the life of the option (5 months). It is unwise for any officer or director to put, or to even appear to put, any limitations on his/her expectation regarding the future value of the company's stock. There should be no conflict or even apparent conflict between an insider and the future growth of the company. Might one be tempted to hold back on an important decision that might cause the stock to rise? Was Bader's sale of the 100 options a bet against the company? Did he have any information which would lead him to expect the value of the stock to fall? No! He simply selected an investment which was going to yield a sure $26,250 over the current market price on the 10,000 shares he had committed. Undoubtedly the absurdness, the cruelty, the shallowness of the "betting against the company" charge more than any other aspect of the incident grated and incensed Bader and drove him to fight the accusation. Technically it is an interpretation, a label, which can be automatically applied to any insider who sells options. But, as is evidenced here, it is an indiscriminate label which can misrepresent the real motivation of the individual. It is like labeling a surgeon who has lost a patient a murderer. Technically he may have performed an act which has taken the life of an individual, hence the label "murderer", but to judge the act without considering the circumstances or the motivation is simply wrong. Bader pleaded his case in the chemical journals and the financial press and gained a great deal of sympathy and support. Articles appeared in the financial columns in American and European newspapers; even a national journal, Forbes, carried a story under the banner "Back stabbing" in which one insider claimed "Cori was tired of working in Bader's shadow and was looking for any excuse to oust him." The company's image among its primary suppliers and customers was tarnished. Numerous leading chemists called, wrote, and took up the case with the CEO at company headquarters. All to no avail.

There is a good chance that an independent, outside chairman would have proceeded more deliberately in his investigation. First, it is unlikely that he would have felt the same urgency to resolve the problem. He probably would have wanted to meet directly with Bader to investigate the incident thoroughly; to review the new legislation, to get the advice of fellow outside board members, of the company's lawyers, and to consider alternatives.

Assuming that one would reserve the severest penalty, dismissal, for the most flagrant violation (a deliberate attempt to take advantage of insider knowledge for personal gain), the Chairman might have considered a range of alternatives: Removal of the "Chairman Emeritus" title; payment of a fine to the company (say some multiple of the alleged insider profits) over and beyond any disgorgement required by law, a public apology to the shareholders, or it might have amounted to nothing more than a slight slap on the wrist with a sharp warning never to do it again. Assuming one of the other alternatives was selected by the Chairman of the Board he would have preserved for the company's benefit one of its most important human assets and continued to reap the rewards from the lifetime association of the company with one of its founders and spokespersons. The Chairman's challenge was to find the "win win" solution which best served the interests of the company; to bet with the company. With an outsider as Chairman, the Board at least would have had the possibility of another option to consider. One outcome is certain: The confrontation between three American businessmen at the Russell Hotel in London on November 20, 1991 would not have taken place.

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

A Chemist Helping Chemists

June 14, 1996

Professor Istvan Hargittai
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Professor Hargittai:

Thank you for your letter of May 28th to Dr. Bader.

He and Mrs. Bader are presently on the Continent, returning to England June 22nd through the end of July. I am forwarding a copy of your letter to him in England, and he will reply personally upon his return to Milwaukee.

Best wishes,

Cheryl Weiss
Office Manager

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4051, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred: May 28, 1996

Thank you very much for your kind letter of May 15. In the mean time I was pained to hear about your difficulties with our magazine through some friends via Israel. This puzzles me a great deal because I had the impression that we were having the most wonderful cooperation. You were very kind to let us print your award address, we are planning to run a brief notice of your book, an article is being prepared for printing in one of the future issues by Dr. Buchan that you had so kindly organized for us. In addition, I am working on the transcripts of our conversation which is bringing back fond memories of our visit. It's true that we have had some difficulty in determining the correct place for a Note by you on Loschmidt. Here, however, I hasten to say that I carry full responsibility for the fate of any manuscript. I may be consulting others, and I usually do, but I never relegate decisions to others be that the Stamp Corner Editor or the History Editor or The Cooking Chemist Editor, etc. So, what is my problem with the Loschmidt piece as it stands? For the Stamp Corner the problem is that at least so far we have had more extensive articles describing areas for which then there was a bundle of stamps. This may and may not be the best practice, of course, and we don't have to stick to it at all. The question at this time would be whether we delay a more extensive article but, again, I see no conflict because we need not be very precise about papers including information about a stamp to appear necessarily in the Stamp Corner. We have already printed information and even pictures of stamps outside the Stamp Corner. So this brings us to the question of the Note format. Here my question is whether the Note contains new information about Loschmidt or not. I am not very knowledgeable but others are telling me that you may have published these observations elsewhere. I can't check this and I'll be satisfied if you tell me that this Note contains new information warranting its publication. If this is the case, the only thing needed would be to reformat the manuscript, bringing references to a reference list, giving figure captions, and use it as a Note. There should be no problem with that.

I very much appreciate your kind cooperation.

With kind regards,

Yours sincerely,

May 30 - June 17 (Italy, Spain)
October 7 - 12 (Sweden)
August 10 - for the 1996/97 academic year (USA):
Dr. Istvan Hargittai, Distinguished Visiting Professor
Department of Chemistry
University of North Carolina at Wilmington
601 South College Road
Wilmington, NC 28403
Fax (910) 962-3013, E-mail hargittai@vxc.uncwil.edu
(Please, use the Wilmington addresses after August 10 only)

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

A Chemist Helping Chemists

August 5, 1996

Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
University of North Carolina
601 South College Road
Wilmington, NC 28403

Dear Istvan:

Enclosed please find the note on Loschmidt, rewritten, I hope, as you require it.

Last month, I sent you by insured mail from England the two Aldrich reprints required for the two figures. I do hope that you received these, but in any case, now also enclosed are Xerox copies of their covers.

I have also received the draft of your interview with me, but that requires a fair amount of work. Could you please give me a deadline, hopefully a few months from now? As you will imagine, my desk is piled high with work accumulated during the last two months.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Enclosures

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

May 14, 1996

TO: Professor Istvan Hargittai
Budapest Technical University
FAX: 36-1-463-4052

Dear Istvan:

Thank you for your letter of May 6th and the galley of the review of my autobiography.

The publisher of the book is Weidenfeld & Nicolson in London. Lord Weidenfeld probably doesn't see book reviews, but if he did, he might object to being referred to as 'Weinfeld'.

Would it be possible also to mention that the book is distributed in the United States by Trafalgar Square?

Do you have any idea why your stamp editor refused to write about the Loschmidt stamp? Will you be able to publish my account?

Isabel and I will be in England from May 26th to June 2nd and then on the Continent until June 22nd. Then we will again be in England until July 26th and in Milwaukee all of August. I would love to be able to chat with you while you are at the University of North Carolina in Wilmington and would appreciate your telephone number.

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

AB/cw

TRANSACTION REPORT

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4051, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred: May 6, 1996

I just sent you a letter when received one from you, of April 30. Many thanks.

Professor Buchan's paper had been typeset and we just corrected the galleys. It won't make the July issue but will certainly be making one of the nearest issues. We have some backlog and try to squeeze in as much material as possible in every issue. I had written a brief review of your book for the previous issue but it didn't make it. The composition of Contents comes from many sources although I am trying to have the upper hand in it.

I very much appreciate your kind cooperation.

With kind regards,

Yours sincerely,

PS I'll be away May 7-21 (USA) and May 30 - June 17 (Italy and Spain), then from mid-August Magdi and I'll be spending the next academic year at the University of North Carolina at Wilmington.

PPS I'm working on the transcripts of our conversation.

I.

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

chemistry, and both chemists and nonchemists will benefit from reading it.

Adventures of a Chemist Collector

BY ALFRED BADER

WEINFELD AND NICOLSON: LONDON, 1995. 288 PP. £ 14.99. ISBN 0-297-83461-4

Alfred Bader is known to many chemists, and Aldrich, the chemical company he created, is known to many more. Bader also has a long list of publications in the *Journal of the American Chemical Society* and other periodicals. Yet today Alfred Bader functions as an art dealer. The history of his extraordinary life is told in this book. He was born in 1924 in Vienna to a unique combination of a Catholic countess mother and a Jewish father, fled to England in 1938, and was interned in 1940 and sent to Canada. He was released in 1941, studied at Queen's University, did his Ph.D. work at Harvard, and started Aldrich in 1951. Bader built Aldrich in a personalized way, making friends with many of the best chemists of his time. On one occasion, when Kodak complained about small orders, Bader advertised for Aldrich, "Please Bother Us." His ouster from the merged Sigma-Aldrich Company, of which he is still a major stockholder, will be the subject of a forthcoming article in this magazine.

Bader made Aldrich very successful. He also collected rare chemicals as other people collect stamps or as he himself collects old masters. Aldrich also made him very rich, and he has engaged himself in philanthropic activities with as much, or even more, dedication as he devoted to any of his other activities. This is an interesting book about a fascinating life, and the story, it seems, is far from finished yet.

How to Write and Publish a Scientific Paper. 4th Edition

BY ROBERT A. DAY

CAMBRIDGE UNIVERSITY PRESS: CAMBRIDGE, U.K., 1995. XIV + 223 PP. £ 27.95. ISBN 0-521-55136-6

"When you have finished the experiments and written up the work, the final typing of the manuscript is not important because, if your work is good, sound science, it will be accepted for publication. Right? That is *wrong*." This is a direct quote from the book (p. 82), and Robert Day helps the reader to produce manuscripts that should be accepted. He starts with the most general questions by defining what is scientific writing, and he pays attention to such details as how to phrase the acknowledgments. Separate chapters deal with each of the elements of a manuscript—the title, abstract, introduction, the sections on materials and methods, and the discussion—with special attention to illustrations. He discusses submission of manuscripts, common errors, and various types of publications. There is even a chapter on how to write a book review. A very useful book indeed.

Chaos in Wonderland: Visual Adventures in a Fractal World

BY CLIFFORD A. PICKOVER

ST. MARTIN'S GRIFFIN: NEW YORK, 1995. XV + 303 PP. PAPERBACK $18.95. ISBN 0-312-12774-X

The author is a computer graphics virtuoso who received his Ph.D. from Yale's Department of Molecular Biophysics and Biochemistry. His primary interest is in scientific visualization. In this book, Pickover recounts the story of an imaginary civilization on Ganymede, one of Jupiter's moons. On Ganymede, living organisms come in three varieties: inorganic, organic, and hybrids. The inorganic creatures possess electrorheological blood and semiconductor brains. Some life-forms use inorganic double helices as their basic hereditary molecules. The book is a real playground for Pickover; in one of the sections, for example, he answers mail from readers of his previous books. As expected, the book is copiously illustrated, but not only by the author's computer graphics, some of them in striking bright color, the works of more traditional artists having been included as well.

Exxon Valdez Oil Spill: Fate and Effects in Alaskan Waters

EDITED BY PETER G. WELLS (ENVIRONMENT CANADA AND THE BEDFORD INSTITUTE OF OCEANOGRAPHY), JAMES N. BUTLER (HARVARD UNIVERSITY), AND JANE S. HUGHES (CAROLINA ECOTOX, DURHAM, NORTH CAROLINA)

AMERICAN SOCIETY FOR TESTING AND MATERIALS: PHILADELPHIA, 1995. 955 PP. $55.00. ISBN 0-8031-1896-1

The tank vessel *Exxon Valdez* ran aground on Blight Reef in Prince Williams Sound, Alaska, on March 24, 1989, and spilled almost 11 million gallons (a little over 40 million liters) of crude oil. It was the largest spill to date in U.S. waters, and its acute impact on the environment was severe. The image of oil-sodden birds has been imprinted in the minds of hundreds of millions of people all over the world. The spill initiated not only a huge cleanup but also a lot of research on its impact. This book consists of 25 research papers presented at an ASTM Symposium in April 1993. The introduction gives an overview of the topics, and the concluding chapter deals with the problems of site protection

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

May 15, 1996

TO: Professor Istvan Hargittai
Budapest Technical University
FAX: 36-1-463-4052

Dear Istvan:

I cannot respond to your letter of May 6th intelligently because I lack two facts: (1) Why does Dr. Edgar Heilbronner not wish to write about the Loschmidt stamp in his Stamp Corner? Surely it is a stamp dealing with the work of a chemist, and the fact that it shows cinnamic acid will be of interest to every collector of chemical stamps; and (2) Not knowing why Heilbronner is so adamant, I also do not know why you do not want to use the brief essay about the stamp which I sent you. Of course, that doesn't have to be in the Stamp Corner, and if you yourself would like to make some changes - perhaps to be less hurtful to Heilbronner - please just suggest these changes.

Istvan, I have just written two very long essays about Couper, Loschmidt, Anschütz and Kekulé for the Plenum publication that will include all of the lectures at the Loschmidt Symposium.

Also, I have just submitted a much shorter essay stressing Anschütz's detective work in uncovering Couper's and Loschmidt's chemistry for *Chemistry in Britain*.

Eventually, I plan to write a very detailed discussion centering on Professors Schiemenz's and Rocke's attacks on Wiswesser. That will be a paper with many dozens of footnotes, perhaps suitable for the *Bulletin of the History of Chemistry*, an ACS publication, but surely not for *the Chemical Intelligencer*.

Please do reconsider your request, reformat my two-page note meant for the Stamp Corner - if you feel that is necessary - and then please let me know what the difficulties really are.

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

AB/cw

DRAFT:

THE LOSCHMIDT STAMP
(for *The Chemical Intelligencer*)

One of the most surprising and instructive stamps honoring chemists in this decade is the stamp *(fig. 1)* honoring Josef Loschmidt published by the Austrian government in June 1995 to commemorate the 100th anniversary of Loschmidt's death on July 8, 1895.

In the 19th century, Loschmidt was known as an able physicist, the man who first calculated the Loschmidt/Avogadro Number in 1865.

In 1861, he published a little book *(fig. 2 shows Aldrich reprint)* giving the structural formulae 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 19th century ever referred to this book.

Then around 1910, Kekulé's former secretary and his successor as professor of organic chemistry at the University of Bonn, Richard Anschütz, discovered Loschmidt's book, which by then was already very rare. Anschütz was astounded: In 1861, in the very year that Kekulé had published his opinion that one could not depict structural formulae, this unknown Austrian had published several hundred structures, many of them correct and clear. The first-day postmark *(fig. 3)* showed one of these, acetic acid.

Anschütz published an article on Loschmidt [Ber. 45, 539 (1912)] and then went to the enormous trouble of taking Loschmidt's book, reformatting it so that it became very much more readable, and arranged for the publication of the reprint in Ostwald's Klassiker der exakten Wissenschaften *(fig. 4 shows Aldrich reprint)*.

Among Loschmidt's correct structures were those of acetic acid, cyclopropane, mannose, benzene, toluene, phenol, aniline, benzidine, and many others.

M. Kohn [J.Chem.Ed. 381 (1945)] published a long article on Loschmidt's chemical work, essentially abstracting Anschütz' paper and notes published with the reprint.

Besides that, few chemists knew anything about Loschmidt's chemical work until William J. Wiswesser of the Wiswesser Line Notation published a startling article [*"Johann Josef Loschmidt (1821-1895): a forgotten genius"*] in the *Aldrichimica Acta* 22 [1], 17 (1989).

That 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 articles have appeared describing Loschmidt's work as a chemist, and from June 25-27, 1995, the University of Vienna held a Symposium honoring Loschmidt's memory. Among the eminent chemists speaking at that Symposium 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.

The postage stamp honoring Loschmidt shows below Loschmidt's portrait the structure of cinnamic acid, one of the many aromatic structures depicted correctly by Loschmidt in 1861. Chemists will note that this was published 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 did not show Loschmidt's greatest achievement in physics, the Loschmidt Number. Unfortunately, the value of the stamp - AS 20 - is very high, yet is of such importance that it will surely interest every serious collector of stamps related to chemistry.

BUDAPEST TECHNICAL UNIVERSITY
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Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred:

May 6, 1996

I would like to suggest to you to prepare a Note, not part of the Stamp Corner, on Loschmidt, using the first day cover as an illustration. It would be nice to have a piece which would differ from your other writings on Loschmidt, may be new facts, may be just a different angle, or even including the reactions by people to your earlier articles. It may also be that more could be written about Loschmidt and less about the Kekule controversy. But this is entirely up to you, of course.

I very much appreciate your kind cooperation.

With kind regards,

Yours sincerely,

PS I'll be away May 7-21 (USA) and May 30 - June 17 (Italy and Spain), then from mid-August Magdi and I'll be spending the next academic year at the University of North Carolina at Wilmington.

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

Dr. Alfred Bader
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A Chemist Helping Chemists

December 27, 1995

Professor Istvan Hargittai
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Istvan:

Isabel and I have just returned from six weeks in England and found your most interesting letters of November 28th to Professor Buchan and November 30th to me.

My letter to Professor Buchan will be self-explanatory. The only rather important change that I would like to suggest is to the last paragraph relating to "disgorgement". there was no alternative punishment, such as a fine, say of some multiple of the alleged insider profits over and beyond any disgorgement, because there never was any disgorgement. I had promised Queen's that I would give them the optioned shares and instructed my stockbroker to transfer the money to Queen's, not to me.

All in all, I find your condensation very fine indeed, and most readable.

I am happy that you will be using my Parsons Award address on Chemophobia. Will you be able to send me galleys for minor corrections?

To turn now to your important questions on the second page of your November 30th letter:

Isabel and I, like my son in the Helen Bader Foundation, try to focus our efforts in a few areas where we feel that our help can really make a difference. With the Helen Bader Foundation, that has been with Alzheimer patients, education (both here and in Israel) and children at risk.

With Isabel and me, it has been to help chemists and art historians in this country, Canada, Britain and in the Czech Republic. Of course, sometimes events overtake the best-laid plans. Such is the case with the many thousands of innocent victims in Bosnia and the enclosed will explain what we are trying to do there.

Hopefully, you and Magdalena will meet with us again, and I will be happy to discuss all this with you in detail. This is so much easier to do personally than through letters which can be misunderstood so easily.

One of the highlights of our 1995 was getting to know the two of you. Please accept our sincere thanks for your thoughtfulness and our best wishes for 1996.

Sincerely yours,

AB/cw

Enclosure

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of **Institute Dr. István Hargittai, Professor of Chemistry**
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Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred:

July 2. 1996

Thank you very much for your kind fax letter of June 23. I hope this message finds you both in good health and that it does find you in the first place. I truly appreciate your suggestions regarding the Loschmidt piece. However, let's keep the possible review and your Note separate. That is, I would like to have your note as a Note in the magazine. On the original manuscript you wrote DRAFT and I take it that you would not mind slightly rewriting it. I would like to suggest two kinds of change. One is, if possible at all, concerns the general thrust of the paper in that it was originally meant for the Stamp Corner but I would rather have it among the Notes. The other is the way references are referred to, and I would like to ask you to number them and have a References list at the end. Concerning the illustrations, everything is fine and in place but the first (Figure 2) of the two copies of the book title pages as republished by Aldrich does not seem to be a very good copy (Figure 3). I trust that you could arrange for a better copy. I take it that you don't need it ASAP and the original first day envelope to Springer when everything gets together. They are good and careful in handling such materials but sometimes awfully slow in returning them, at the end though they always come around.

There is no haste about this manuscript as I realize that being in England you may not have all what is needed at hand. I am doing this letter only because I feel that this has been stretched rather long and this is just a token of my appreciation of your courtesy.

I very much appreciate your kind support.

With kind regards

Yours sincerely

Alfred Bader
Milwaukee, Wisconsin, November 8, 1995

István Hargittai (IH): I would like to ask you about your chemistry. Not only did you create the famous company Aldrich, found *Aldrichimica Acta*, and build up a remarkable art collection, but you have also done considerable research in organic synthesis.

Alfred Bader (AB): I first became interested in research in my senior year as an undergraduate at Queen's University. There was a very good teacher, Professor Norman Jones, a famous spectroscopist. He allowed me to do a research project which I enjoyed. Then I got a very fine job with a paint company in Montreal, and a year and a half later the President of the company suggested that I go on with my studies and offered me company support. I did my Ph.D. studies at Harvard in 1947-1949 with Louis Fieser, who traveled so much at that time that his students saw very little of him. But there were many able chemists, students and faculty, who were very helpful.

Louis Fieser simply said to me, *'Here's a quinone; in alkali it turns red, overnight it turns yellow. Find out what happens.'* A year and a half later, he came into my lab and asked me *'How is that project going?'* I said I'd solved it. Fieser said *'Give a seminar.'* He was satisfied, said, *'write it up for a paper'*, and there it was. So all went well, but I realized one thing: I was not a world-class chemist. I was a very good experimentalist, but there were many things I didn't understand in theoretical chemistry.

I felt obligated to go back to the paint company in Montreal, but it had been bought by the Pittsburgh Plate Glass Co. whose paint research was concentrated in Milwaukee. So that is how I came here in January 1950. The company gave me a job but had no idea what to do with me. All the research they did was in oil chemistry - linseed oil, soybean oil - and here was a Ph.D. chemist from Harvard trained in synthetic chemistry. But they left me alone, and I got interested in producing monomers from inexpensive starting materials - phenol with butadiene, cyclopentadiene and isoprene, for instance. The literature said that chemists had tried the reactions and they didn't work. But I found that if I controlled the catalyst concentration carefully, I could make them work. We had a whole new series of unsaturated phenols, easily made from starting materials costing pennies.

One day a salesman from Quaker Oats stopped by and said that levulinic acid would soon be available very inexpensively from Quaker Oats. The moment I heard that, I made the bisphenol reacting levulinic acid with phenol to make what is now called diphenolic acid. A few weeks later, I sent a note off to JACS. Soon Johnson Wax wanted to buy the patent for which we had applied. Our Director of Research asked me, *'What should we charge for this?'* I said,

'It was two days' work; if we got ten thousand dollars, we would be well paid, but they must want it very badly, so ask for a million!' Well, he got it. Then, of course, lawyers descended on my lab to make sure everything I worked on was really patented, but I had already seen to that.

In 1954, PPG decided to move their paint research to Pittsburgh, but I didn't want to go there, left the paint company and devoted full time to Aldrich. Shortly after arriving in Milwaukee, I had asked my director of research whether he would allow me to start a small fine chemicals division. At that time, Eastman Kodak had a monopoly, but offered only 4,000 compounds. I thought we could easily make 250 compounds a year that were not in the Kodak Catalog. I was told that PPG was not interested; nobody could compete with Kodak. Yet today Kodak is no longer in the fine chemicals business. I felt that Kodak was not doing a good job and that chemists would be glad to have another source. So a lawyer friend and I set up a small company, Aldrich, very much a weekend operation with a capital of $500.

In the mid-1950's, when I visited customers, they would say, *'Aldrich, you're the cheap people.'* Kodak was very expensive, and they didn't really care about their fine chemicals business. They even had an ad in which they admitted that their service was poor. As a response, we published an ad saying *'Please bother us! We hope we never get so big that you can't talk to us.'*

IH: You've built up a library of chemicals. Where is it now?

AB: At Aldrich. It's close to a hundred thousand compounds. We have many famous chemists' research samples. For instance, Louis Fieser's, Bob Woodward's, Tadeus Reichstein's, you name them. A great many good things have come out of this library. Suppose that a medicinal chemist has an idea that a given bromolactone has some medicinal effect. He can contact Aldrich and get a computer printout of every bromolactone and order whichever he wants at $40 a sample.

Some years ago, a medicinal chemist in California, Dr. Summers, believed that acridines might help in the treatment of Alzheimer patients. He asked for our list of acridines, ordered some of each, and then came back wanting a hundred grams, then a kilo, then 10 kilos of one particular acridine. Years earlier, a Viennese chemist, Dr. Pickholz, working in London, had said to me, 'I've got this acridine, aminotetrahydroacridine; I think it's important in brain chemistry, I don't know how, but take a little, and we'll teach you how to make it'. For years, there was little interest in it until Dr. Summers came along. The rest is history: THA was, I believe, the first drug licensed by the FDA in the treatment of Alzheimer's disease.

IH: Should there be a universal library of all compounds?

AB: If there were a universal library, it would be run by some government agency, and it would be much more cumbersome to get samples. With Aldrich, it's very simple. It used to be called the Alfred Bader Library or the ABC Library, but when I was thrown out of the company, they dropped the Alfred Bader. Even ABC was too close; it's now called the Sigma-Aldrich Library, but it's still the same. Sales now exceed two million dollars a year, with many thousands of samples going out.

IH: What are the criteria for a compound to get into this library?

AB: It must not be in the Aldrich Catalog, and it must be clearly labeled. We don't analyze for the library, but we buy only from reputable researchers. Maybe two or three percent of the compounds are not what the researcher thought 20 or 30 years ago, and about 10% are not very pure.

IH: You said you didn't want to be so big. Why then did you merge with Sigma?

AB: It seemed to me in the late 60s, early 70s - but now I think I was mistaken - that organic chemistry had peaked. Woodward had synthesized strychnine; what more was there to do? This was before I really understood H.C. Brown's hydroboration. This was before Barry Sharpless' epoxidations. There's so much that has been done since. But I thought that most of the research funds would come to biochemistry and biomedical applications. I visited Sigma in St. Louis in the late 60's and proposed a merger, and they almost threw me out physically. Then Sigma went public in 1972, had some bad publicity and its stock dropped from 22 to 11. They were very thin in top management. At that point they listened to me, and the merger has been very good for everybody. Only Dan Broida, the head of Sigma, was against the merger. He was very dictatorial, but immensely hard-working, and you could call him day and night, collect. He had built Sigma sales to about 30 million dollars a year. Our combined sales then were about 45 million dollars. This year the sales of Sigma-Aldrich will be close to one billion dollars.

IH: You are still a stockholder; does it give you any say in company matters?

AB: I'm the largest individual stockholder, but it doesn't give me any say whatever.

IH: For decades you've been visiting synthetic chemistry laboratories in the best universities. Can you share some of your experiences with us?

AB: I don't see great differences among the countries where I used to go. Funding is very much more difficult in Britain than either in Germany or in the United States. The laboratories, the equipment are very much better in Germany and in the United States than in Britain. Comparing 1995 with 1950, a good chemist today could finish my Ph.D. work in a month. It took me a year and a half. There's so much more equipment around now. Then, NMR was unknown, and there was no mass spec. We had an infrared at Harvard, it was a big instrument and was on the blink 20% of the time, but it worked. It was amazing to listen to Bob Woodward or Gilbert Stork interpreting the spectra.

Today synthetic work can be done in so much smaller quantities than then. In our library of research chemicals, I can tell by looking at Woodward's students' bottles about when the compound was made. In the 1940s, 1950s, you had gram quantities; in the early 70s, you had hundred milligram quantities. Today 5 or 10 milligrams suffices.

IH: How about the image of chemistry?

AB: There has been a tremendous change, much for the worse. If you had gone to Harvard Square in 1947 and asked people on the street, *'What is your first reaction to chemistry?'*, they would have said, *'vitamins, new plastics, new drugs'*. Do it today and they answer, *'pollution and carcinogenic chemicals'*. We have not done a good job pointing out how much chemistry does. This is terrible - not for chemistry but for the world. When young, brilliant students see, for instance, the world sinking into a cesspool of toxic chemicals on the cover of *TIME* magazine, why should they want to become chemists? We rely on the media, and the media have done badly. I remember a headline in the *Milwaukee Journal* saying *"Benzene found in a well near chemical company"*. But the details in the text were that two parts per billion of benzene had been found. This is crazy. It's next to nothing. Our analytical ability has changed so that today we can show that everything is everywhere.

It's also true that there have been chemical industries that have done very wrong things, and then tried to hide them. The word *chemistry* has become an ugly word, but everything is chemical.

IH: About *Aldrichimica Acta*. To how many addresses is it delivered?

AB: It's free of charge, of course, and it goes to about 200,000 scientists worldwide. We have had very good papers in it. Over the years, we have established a number of awards in America, Canada, Britain and the Czech Republic. We used to ask the award winners to submit papers on their award addresses.

IH: Is there any connection between your collecting chemicals and collecting paintings of Old Masters?

AB: These are completely separate matters. Take the chemicals first. No chemist wants to throw out his research samples. Unfortunately, when a professor dies or retires, these are often discarded. I could tell you story after story. For instance, Professor Hawarth's compounds at Birmingham. I feel so unhappy thinking about this every time I go to Birmingham. Here were thousands of his crystalline sugars, so difficult to crystalize. Some bureaucrat got worried, and they put many of these samples together into biscuit tins, poured in cement and threw them out. Imagine the idiocy of throwing out these crystals because some fool was afraid of these sugars!

Some years ago we went to Ames, Iowa, where all the Henry Gilman samples were stored in one big room, thousands of them. A company wanted $8,000 to remove them. I offered to pay for the chemicals and send a truck to pick them up. The only mistake we made was that the truck we sent wasn't big enough so we had to send it twice. There were 20,000 bottles. We immediately discarded about 12,000 because these were chemicals which Aldrich listed. There were another few thousand where the labels had fallen off or the materials had decomposed. We were still left with 3,000, and we published a little yellow catalog of the Gilman samples, just as we published a blue catalog of Woodward's samples.

About collecting paintings, when I was a kid, I lived in a home surrounded by paintings, but they were modern Austrian, and I didn't like them. In time, I realized that I liked Dutch historical paintings and Dutch portraits best. In the early 50s, I started buying pictures that I liked and that I could afford. Today I'm a dealer as well as a collector. I buy about 200 paintings a year. Last month I bought a very fine Rembrandt and yesterday I bought a beautiful TerBorch, probably the best outside of a museum. But I'm trying to have a non-elitist gallery. I have many pictures here from a hundred dollars up, and on the other hand, the Rembrandt is several million. I spend about a third of my time buying and selling paintings, another third writing, and the remaining third working with chemical companies. I invest in them, consult and advise them. I'm trying to find customers for them and suggesting new products. I just bought a ten-percent interest in a large but very ailing English company called Anglo United, which owns Coalite. I know Coalite Chemical very well, and I think I may be able to help them.

IH: Do you now do 100% what you like to do?

AB: Yes. I'm far happier today doing what I'm doing than I was four years ago. Then I had to work with the top management of Sigma-Aldrich in St. Louis. In the hundreds of meetings in hundreds of days in St. Louis, there was never a day that I really enjoyed myself there.

IH: What do you miss from those days?

AB: The most enjoyable part of my work was the 50% when Isabel and I simply walked from lab to lab, talking to students, asking them, *'What are you making that Aldrich should be offering? What do you need? What should we add to our catalog?'* My last such visit was early in 1992, before I was thrown out of the company, and I really miss those visits.

The most productive were to the top schools. We realized early on that 90% of the best research is done in 10% of the universities.

We would spend a most enjoyable day on the sixth floor of Chandler at Columbia University, for example, talking to each of the Gilbert Stork students, learning what they were doing and what they needed. Then a year or two later, I'd meet the same students as post-docs at the ETH or Cambridge, and two years later they'd have their first Assistant Professorship at an American university. It was a wonderful give-and-take. I was far better at that than I ever was as a research chemist.

IH: You give a great emphasis to your being Jewish in your autobiography. But you are Jewish by choice. You might have become Catholic, following your mother's side of your family.

AB: I was adopted by my father's sister, a Jewess. I also studied Judaism. At the time of the *Anschluß*, I was a boy of 14 in Vienna and saw all the propaganda of how terrible Jews were. I asked myself the question, *'What if these people are right?'* So I felt I had to study Judaism, and it became clear to me that the Nazis weren't right. I'm a convinced Jew and my two wives, Danny and Isabel, who came from religious Protestant backgrounds, became convinced Jewesses.

Coming back to the question about my Catholic mother, I hardly knew her. She would come once a month to the house, and occasionally she would say, *'Bobby [as I was called then], anyone who could be a Catholic and isn't is going to go to Hell.'* I didn't really know her as a person. I very much wanted to visit her in October of '47. She was then very sick and I asked Louis Fieser for three weeks off. *'No'*, he said, *'if you go, you'll lose your fellowship. Go next summer.'* Sadly, my mother died in April of '48.

IH: Referring to your two interests, what do you find common between chemistry and art?

AB: First of all, there is the restoration of paintings. This relies heavily on the knowledge of chemistry. Secondly, for hundreds of years, artists have tried to create something beautiful. Many artists today are desperately trying to create something new. They often use chemistry in their search for new materials.

People often ask me whether I restore my own paintings. I never do. When I buy a dirty old painting, I determine whether there is much nicotine on it. Often just saliva will take off a lot of dirt and nicotine. But I stop at that point and work with two very competent restorers. I have just acquired a painting which may be a late Rembrandt, with a terrible varnish. The restorer will clean it and then we'll know better.

The restorers have to choose the right solvents, which usually take off the varnishes easily. The cleaning has to be done very carefully, and it may take a very long time. Often there is overpaint that has to be removed. Today we realize that all restoration should be reversible, but it wasn't so 200 years ago. Today competent restorers do inpainting over an easily removed varnish. Years ago, restorers often painted oil on oil. Almost all paints were based on linseed oil, which takes three or four hundred years to polymerize completely by oxidation. If a painting of the 16th century was overpainted in the 17th century, that overpaint has also polymerized and is very difficult to remove.

When I say overpaint, I'm not speaking of painting a new picture over another one. In the past, paintings were not so valuable, and possible damages and paint losses may have been corrected in an unprofessional manner. The restorers may just have been house painters, who overpainted much more than was needed. I have seen a little book, published in London in 1752, entitled *How To Be A Butler*. It advises that if the master has a dirty painting, the butler should take a bucket of wood alcohol (i.e. methanol) and a sponge. This would take off the dirt, but also the varnish and the top of the paint layer. There are so many paintings that have been skinned because the top layers have been removed.

I like nothing better than to find a 17th century painting to which nothing has been done. After 400 years, the polymerized paint film is practically indestructible, so the paint film holds the canvas together. But most paintings have been relined because over the years the canvas became as brittle as old paper. Restorers came along and backed the original canvas with a new canvas, putting glue in between. They'd put the painting face down, add a layer of glue, and the new canvas. Then they would use a hot iron to make sure that the new canvas adhered to the old. But when you do that to a thickly painted picture, the paint film gets flattened out, and this is terrible. Today, of course, competent restorers, if they have to reline, do it on a vacuum table so that the paint film doesn't get flattened out, but it is preferable to avoid relining

altogether.

IH: What was the biggest mistake you made in the building of Aldrich and Sigma-Aldrich?

AB: We had some great chemists, and I didn't treat them well enough financially and they left.

We started the company with a capital of $500, our capital in 1951, and I had to be penny-pinching. This was nothing new to me. I had never had any money, and even now I am still careful on a personal level. I realize that I should have been more generous with our best people.

IH: Was there any question in our conversation that you'd like to return to?

AB: Yes, concerning Aldrich. Clearly, my heart is with the company. I'm very proud of having founded Aldrich. Today research is different from the way it was in 1950 because Sigma-Aldrich supplies so many thousands of chemicals. We've made research very much easier and saved chemists of the world millions of hours that they can now devote to their own research rather than to making starting materials. I'm very proud of what I've done and of the many friends I've made around the world.

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

October 16, 1996

TO: Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
FAX: 910/962-3013

Dear Istvan:

Thank you so much for your seven page Fax.

The article is presented beautifuly; many thanks.

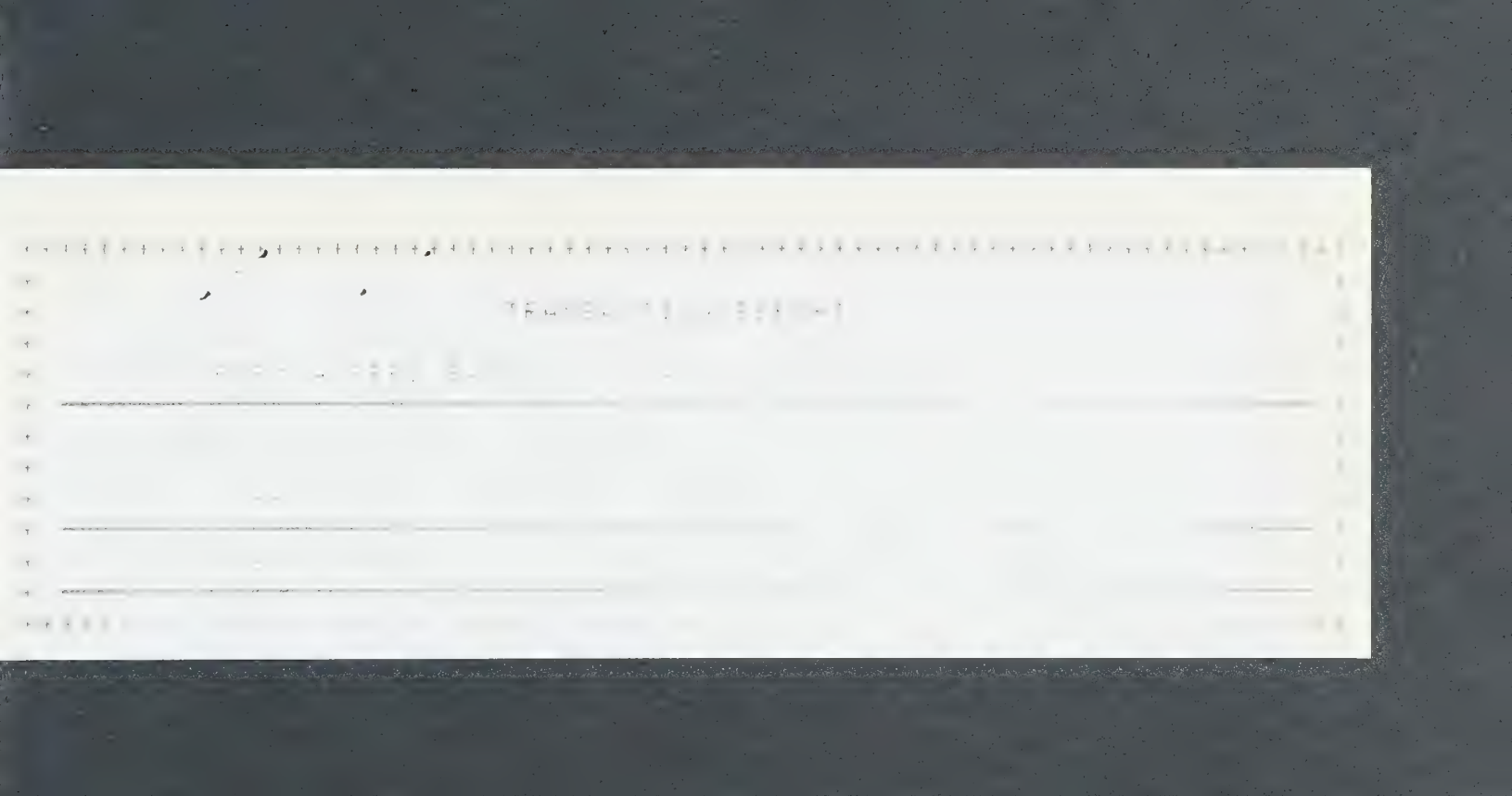
By the time I meet Professor Buchan in Kingston on October 25th he may have the paper; if not I will show him the Fax.

I think that you will find that this article will be read by a great many chemists.

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

Sincerely,

AB/lh



FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

October 15, 1996

TO: Professor Istvan Hargittai
Distinguished Visiting Professor
Department of Chemistry
FAX: 910/962-3013

Dear Istvan:

Isabel and I are planning to leave for Canada first thing next week and also plan to meet with Professor Bruce Buchan.

I had hoped to have the October *Chemical Intelligencer* to show him, but it has not yet arrived. Could I impose on you to fax me just the pages with Buchan's article?

With many thanks for your help and best personal regards, I remain,

Yours sincerely,

AB/cw

UNCW

THE UNIVERSITY OF NORTH CAROLINA AT WILMINGTON

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

September 24, 1996

Dear Alfred:

Thank you very much for your kind letter of September 20. The year-end deadline for the corrections was suggested because you yourself had told me that you were, very understandably, very busy due to your long absence from your office. Thanks for the corrections. The added question was a nice one (I mean, the answer).

Professor Buchan's paper is coming out in the October issue.

We have no plans at this time to travel in the direction of Milwaukee.

Magdi is joining me in sending you both our best wishes.

Yours sincerely,

Best wishes

DEPARTMENT OF CHEMISTRY

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Candid chemistry

Harold Kroto

The Chemical Intelligencer. Editor-in-chief István Hargittai. *Springer. 4/yr. $69 (institutional); North America $29, elsewhere $33 (personal).*

"INTELLIGENCER"? What does this word mean, I wondered. Perhaps the editor, István Hargittai, had actually got hold of the (in)famous Hungarian–English phrase-book (famous at least among Monty Python aficionados) that was originally used by John Cleese to buy matches — among other things. It turns out to mean 'bringer of information', in this case chemical (or chemistry?) information. But why, one might ask, should chemists, who already have a plethora of specialized publications catering to their professional interests, need yet another periodical?

The niche exists because chemists are a peculiar lot. For one thing, I know few who have not developed expertise in some other field, whether the arts, cooking, sport or what have you. I often wonder why so many became chemists when they could have been equally, if not more, successful pursuing their alternative passions — they would almost certainly have been richer.

Chemists also suffer from a curious professional form of schizophrenia: their thoughts are a mixture of abstract and hyper-realistic concepts at one and the same time; they are always subliminally aware that the intrinsic quantum properties of atoms and electrons govern all aspects of our everyday world in a way hidden from others. So the formula of benzene or its smell automatically triggers access to banks of information about the chemical and physical properties of this compound. Yet the general public may be only vaguely aware that benzene is an additive in petrol, if they have heard of the term at all.

There is one other important factor. It is the chip that rests on our communal shoulder: the fact that no-one has done more than chemists to improve the quality of everyday life and yet this contribution goes virtually unrecognized even though it daily stares everybody in the face. We chemists crave belated recognition of our modern Renaissance role.

Chemical Intelligencer covers this idiosyncratic range of interests. There are articles, interviews, notes, book reviews and letters on food, chemistry in Kuwait after the Iraqi invasion, the arts (writing, music, painting, sculpture), symmetry, postage stamps with chemistry themes, molecular models, the laboratory environment, historical articles, famous and infamous chemists (dead and alive), violins, photography — indeed anything that chemistry influences, which does not leave out much in the final analysis.

The quality of the articles is inevitably uneven, but the content is never dull. The magazine is well illustrated and includes a wealth of excellent photographs, diagrams and historically valuable archival material. As it makes its mark — as it undoubtedly soon will — it cannot fail to attract high-quality material. The unmistakable spirit of the editor, who has the charm to extract material — including frank interview revelations — from the busiest of scientists, pervades the pages.

There are as many different types of chemist as there are chemists, but I suspect that most would enjoy subscribing to this inexpensive, idiosyncratic but invariably fascinating publication. □

Harold Kroto is at the School of Chemistry and Molecular Sciences, University of Sussex, Falmer, Brighton BN1 9QJ, UK.

Rising to the top

David A. King

Current Opinion in Colloid and Interface Science. Editors E. W. Kaler and B. H. Robinson. *Current Science. 6/yr. $612.50, £370.50 (institutional); $212.50, £130.50 (personal); $98.50, £63.50 (student).*

Adsorption: Journal of the International Adsorption Society. Editor-in-chief K. S. Knaebel. *Kluwer. 4/yr. DFl456, $319 (institutional).*

IT is a rare pleasure to be able to give an unqualified welcome to a new journal. I am delighted to be able to recommend research students and their senior colleagues working in colloid and interface science to subscribe to this new *Current Opinion* journal. The format has proved very successful in the biological and medical sciences, and there is clearly no reason why this should not also be the case in the physical sciences.

The formula is relatively simple. The whole subject matter covered by the journal is divided into 12 sections, and each section is to be covered once a year by short "subjective" reviews by experts working in the field. These reviews are usefully supplemented by bibliographies of relevant papers in the published literature, with the papers "of special interest" awarded one star (or bullet point) and those "of outstanding interest" two. I can think of no easier way of keeping abreast of the whole field than to browse through each issue, but the journal has archival value too. These reviews and the bibliographies will become indispensable to all future writers of reviews, chapters or monographs in colloid and interface science.

The true measure of the success of the journal, and hence the editors, lies in the status of the reviewers who have been attracted for the first volumes. The list of section editors and their reviewers reads like a *Who's Who* of the field.

The topics have been well chosen, too. So far this year the following sections have been covered, each consisting of an overview by the section editors followed by between 8 and 12 subject reviews: scattering and surface forces; experimental self-assembly; imaging and other techniques; material aspects; theory of self-assembly; and thermodynamic and theoretical aspects. In the remaining three issues this year we are promised: rheology and rheological techniques; applications in chemistry and chemical engineering; surfactant science; colloidal aspects of biotechnology, biochemical engineering, pharmaceuticals and synthesis; dynamic aspects of colloids and interfaces; and food colloid emulsions, gels, foams and aerosols. The journal is well produced, in a good, easy-to-read format, and the editors, who must be working overtime to keep their deadlines, must be congratulated on the overall high standards they have established.

Adsorption is quite another matter. I have worked in the field of chemisorption for some 35 years, and so was surprised to discover that there is an established International Adsorption Society of which I knew nothing. This is the new house journal of the society, and, looking through the first few issues, I was unable to discover a distinctive flavour; is it trying to cover too much?

Most of the papers are from researchers in chemical engineering, dealing largely with the macroscopic properties of adsorption phenomena. This is clearly an important area. It bears little relationship to the detailed studies using spectroscopic and imaging techniques on well-defined single-crystal surfaces, with which I am more familiar, and this clearly explains my lack of familiarity with the society. A "Special Issue" does however cover molecular modelling of adsorption, indicating a wish to spread from applied to fundamental science. But there are good, well-established specialist journals that deal with these areas of adsorption studies, such as *Langmuir* and *Surface Science*. I am not convinced that the case is made for this addition.

I found the presentation irritating, even childish: oversized figures, many with the appearance of overheads prepared for seminars, with grossly oversized printing. Some good papers have been published in the first four issues, but I am not convinced that leading scientists in the field would send their best work here. □

David King is in the Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK.

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4051, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

To Prof B Buchan

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

Dear Alfred:

February 16, 1996

Thank you very much for your communications. In the meantime both you and I have received the missing last lines of your award address. Everything seems developing fine. I am scheduling your award address for the next issue, and I am very pleased to be able to bring it out so quickly.

In the meantime Dr. Buchan has also finalized his submission and added three sample illustrations from the covers of the ALDRICH catalogs. I think they'll enliven the text nicely.

I have mentioned the stamp to the Stamp Corner Editor but he did not seem enthusiastic and said that he was not planning to deal with it in his articles. However, it does not have to be that the Section Editor should be writing all the contributions himself. You could put together a note on the stamp, for example.

It means a lot to me that you like the magazine.

I very much appreciate your kind cooperation.

With kind regards,

Yours sincerely,

cc Prof. Bruce Buchan

Best wishes

Anna

PS I'll be away [USA 2/17-3/10 and Israel 3/28-4/23]

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202
Phone: 414/277-0730
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A Chemist Helping Chemists

April 30, 1996

Professor Istvan Hargittai
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Istvan:

I just received your delightful and multi-faceted *Chemical Intelligencer* of April and noted how well you presented my article on Chemophobia. Many thanks.

Do you plan to publish Professor Buchan's article in your July issue and will you also be using my note on the Loschmidt stamp?

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

Yours sincerely,

AB/cw

BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
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Dr. Alfred Bader
924 East Juneau, Suite 622
Milwaukee, Wisconsin 53202

March 22, 1996

Dear Alfred:

Thank you very much for your kind letter of March 8 with the draft of a Stamp Corner submission. I am sending it on for review to the Editor of the Stamp Corner. I have no idea why he was not interested in the Loschmidt stamp. I agree that it is of interest and to the point.

I am sending only copies of the silver plate and the first day cover, so as to expose them to the least amount of potential damage.

Magdi and I are leaving for Israel March 28 and I'll be back April 23. I don't expect to be able to report to you about the Editor's comments before that.

I very much appreciate your kind cooperation.

With kind regards,

Yours sincerely,

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

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FROM
Agnes BADER
2961 N SHEPARD
MILWAUKEE WI 53211

TO
PROF I HARGITTAI
Inst. of Chemistry
BUDAPEST XI HUNGARY

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

A Chemist Helping Chemists

March 8, 1996
Via Registered Mail

Professor Istvan Hargittai
Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Istvan:

In response to your letter of February 16th, I wish I knew just why your Stamp Corner Editor, Edgar Heilbrunner, doesn't want to write about the Loschmidt Stamp. I really can't think of many stamps dealing with chemistry as interesting as that one.

In any case, I have written a short article, enclosed, which you might like to use. I also enclose Xerox copies of the covers of Loschmidt's books, Figs. 2 and 4, as well as a silver print of the stamp and the first-day postmark, showing acetic acid. I also enclose the list of plenary lectures held in Vienna on June 26th.

Please do let me know if you require anything else for this discussion of the Loschmidt Stamp. I would appreciate return of the silver print, as that is the only one I have.

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

Yours sincerely,

AB/cw

Enclosures

SOME PERSPECTIVES IN MOLECULAR STRUCTURE RESEARCH:
AN INTRODUCTION

István Hargittai and Magdolna Hargittai

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ABSTRACT

Over the past years the accuracy of molecular structure determination has increased. This is due not only to improved experimental and computational facilities, and to the combined application of various techniques, but also to a better understanding of the physical meaning of structural information from different sources. Critical assessment of structural information facilitates its application to investigate intramolecular and intermolecular interactions and their consequences on the rest of the molecular structure. Supramolecular chemistry poses new challenges to accurate molecular structure determination at various levels of complexity of chemical systems.

I. INTRODUCTION

Much of chemistry is structural chemistry. Conversely, structural chemistry is also part of the science of structures. The discovery of the stable C_{60} structure is a case in point.

H. W. Kroto [*1*] describes eloquently how his previous encounters with Buckminster Fuller's work, and, in particular, the geodesic dome of the U.S. Exhibition Hall at the 1967 Montreal Expo, have assisted him to arrive at the highly symmet-

Figure 1. The sphere decorated by regular hexagonal pattern with pentagons inserted here and there. This sphere is found under the paw of a lion-guard in front of one of the palaces in the Forbidden City, Beijing, China (photograph taken by one of the authors in August, 1993).

rical truncated icosahedral structure. This was a lucky synergy. For mathematicians, though, this has been a familiar structure. We quote here from the Introduction of Gasson's *Geometry of Spacial Forms* [2] which appeared on the eve of Kroto's discovery:

> . . it is impossible to construct a faceted spherical or part spherical surface (a dome for instance) if one has but hexagonal panels at one's disposal. There are always twelve pentagonal panels in a completely spherical ball and a set of quanta of hexagons,. . .

For another nonchemical illustration, Figure 1 shows a sphere decorated by regular hexagons with pentagons inserted here and there in the pattern. The truncated icosahedron has 20 hexagons in addition to the 12 pentagons, and it is one of the semiregular solids of Archimedes. All carbon substances whose cage molecules contain 12 pentagons and various numbers (except one) hexagons, are called fullerenes, and C_{60} has the special name, "buckminsterfullerene". What Gasson [2] states about the importance of structure is a truism both in geometry and in structural chemistry: "structural pattern is present in all things. ... The study of geometrical structure is universally all-important". We augment this with Kepler's succinct statement, "Ubi materia, ibi geometria" [3(*a*)].[1]

II. THE IMPORTANCE OF MOLECULAR GEOMETRY

The hypothesis of the truncated structure for the remarkably stable C_{60} molecule was followed by infrared [4] and NMR spectroscopic [5] evidences for molecular shape and symmetry. However, the ultimate proof of the structure came with the determination of the molecular geometry of buckminsterfullerene (Figure 2). Table 1 has the bond lengths from different techniques [6–9].

Molecular geometry is determined by the relative positions of the atomic nuclei in the molecule. It is most conveniently described by the so-called internal coordinates, i.e., bond lengths, bond angles, and the angles of torsion.

Let us use some quotations on the importance of determining the geometry of molecules. The first one is from a book on the story of polywater by Felix Franks [10]:

> The central problem in the identification of a new chemical compound is the determination of its molecular structure, the linkage structure of the various atoms in the molecule, the length and strength of the bonds between the atoms, and the general shape of the molecule. This type of information is basic to an understanding of how such a molecule can interact with other molecules, how it takes part in chemical reactions, how the substance crystallizes on freezing, and how the molecules might interact in the liquid state.

The added importance of this quotation is that molecular structure was exactly the kind of information that was never obtained (and could not have been) for polywater.

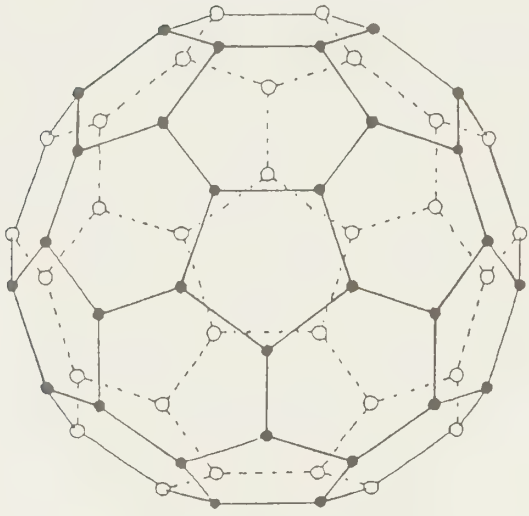


Figure 2. The truncated icosahedral structure of buckminsterfullerene, C_{60}.

Another eloquent, and much quoted, statement is by Roald Hoffmann [*11*]:

> There is no more basic enterprise in chemistry than the determination of the geometrical structure of a molecule. Such a determination, ..., ends all speculation as to the structure and provides us with the starting point for the understanding of every physical, chemical and biological property of the molecule.

Table 1. Bond Lengths in Buckminsterfullerene

Lengths of Shared Edges of Rings	*Gas ED*[a]	*Neutron Crystallogr.*[b]	*X-ray Crystallogr.*[c]	*Ab initio MO Calculs.*[d]
	1000 K	5 K	110 K	
	r_g	$r\alpha$	$r\alpha$	r_e
	1991	1991	1992	1991
C(5)–C(6),[e] Å	1.458(6)	1.455(12)	1.445(5)	1.45
C(6)–C(6),[f] Å	1.401(10)	1.391(18)	1.399(7)	1.39

Notes: [a]Gas-phase electron diffraction [*6*], for r_g, see Section IV.A.
[b][*7*], for r_α, see Section IV.A.
[c][*8*], for r_α, see Section IV.A.
[d][*9*], for r_e, see Section IV.A.
[e]C(5)–C(6) is the bond shared by a pentagon and a hexagon.
[f]C(6)–C(6) is the bond shared by two hexagons.

There is then a recent statement by Marlin Harmony [*12*]:

> ... surely the most characteristic attribute of a molecule is its three-dimensional structure, i.e., the geometrical arrangement of its constituent atoms. There can be no doubt that the development of chemistry in the 20th century has been paralleled, if not led, by advancement in our quantitative knowledge of molecular structure.

Two succinct but powerful statements are the following, one by C. A. Coulson [*13*]: "No one really understands the behaviour of a molecule until he knows its structure that is to say: its size, and shape, and the nature of its bonds." The other is attributed to Linus Pauling: "The most important characteristic of a chemical bond is its length."

It is to be stressed, of course, that the geometry of the molecule is only one of the three major aspects of molecular structure. The other two are the *intramolecular motion*, which comprises the relative displacements of the atomic nuclei with respect to their equilibrium positions, and the *electron density distribution*. Furthermore, molecular structure is only one of the characteristics structural chemistry is dealing with. Since our introductory chapter deals primarily with molecular geometry, it covers only a relatively small, though fundamentally important segment of structural chemistry. Various aspects of molecular geometry are also discussed in other chapters in this volume along with other characteristics of molecular structure and other branches of structural chemistry. We are aiming at the broadest coverage of structural chemistry over the years in this and future volumes.

III. LOOKING BACK

Perspectives mean not only the future but the past as well. We find it prudent to review the origins of structural considerations in chemistry. Here, however, we are going to mention only a few important moments without any attempt to be comprehensive. We have already quoted Kepler [*3(b)*] who first considered packing as he was examining the beautiful snow crystals. The atomistic views date back, of course, to the Greek philosophers of whom Democritos (460–370 B. C. E.) stated: "Nothing exists except atoms and empty space; everything else is opinion" [*14*]. It is also noteworthy that the representation of the internal structure of snowflakes by Kepler, as densely stacked balls (Figure 3), appeared 200 years before Dalton and 300 years before X-ray crystallography began. Close packing was also invoked in Dalton's papers (Figure 4) as he was illustrating his views on gas absorption [*15*].

Looking back, some historical facts may appear in a different light today than they did yesterday. As science progresses, the relative importance and the significance of some discoveries may change. Avogadro's law has been a basic tenet for a long time in chemistry: "Equal volumes of all gases at the same temperature and pressure contain the same number of molecules." However, to Buckminster Fuller, Avogadro's law was more than what is stated literally. He saw in it a proof that

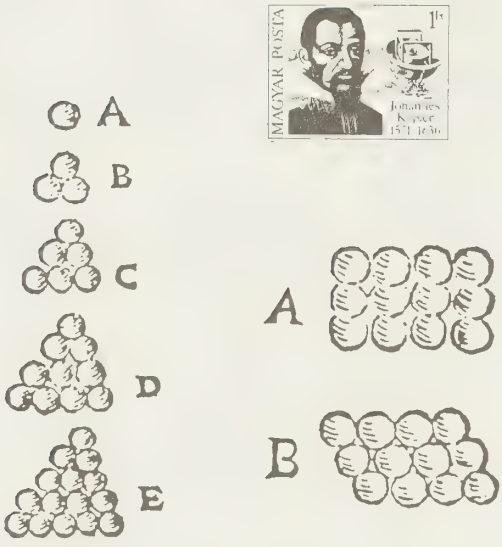


Figure 3. Closely packed spheres by Kepler [*3b*].

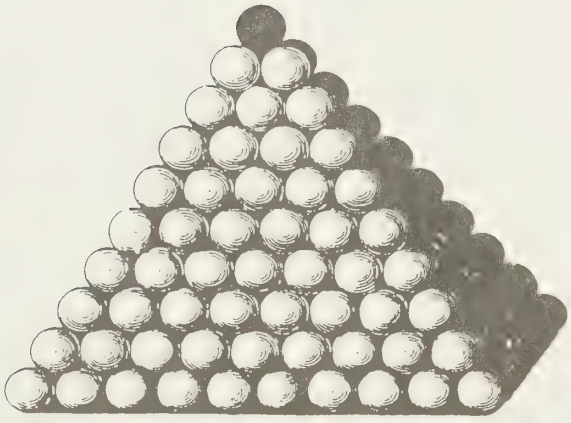


Figure 4. Pictorial illustration of gas absorption by Dalton [*15*].

chemists considered volumes as material domains and not merely as some abstractions [*16*]. This was important to Fuller as he advocated a physical kind of geometry and found an especially synergistic science in chemistry.

In today's world of ever-increasing importance and penetration of computational chemistry, it is instructive to quote Gay-Lussac [*17*]: "We are perhaps not far removed from the time when we shall be able to submit the bulk of chemical phenomena to calculation." This statement is not only remarkable for its prescience but to us it is also a caveat. Today we are closer to Gay-Lussac's target by more than a century but it is still far away for many purposes.

The most immediate roots of structural chemistry are in the well-known works and discoveries of Pasteur, van't Hoff, and others [*18*]. The four valences in a tetrahedral arrangement of carbon, however, were first described by Emanuele Paternò [*19*] in an obscure journal. Since he did not develop all the consequences of his hypothesis, the credit, justifiably, belongs to van't Hoff (and Le Bel). Yet it is worthwhile to quote Paternò (after [*20*]) because there is even direct reference in his work to what would be called conformational isomers today:

> ... one of the fundamental principles of the theory of the constitution of organic compounds, based on the atomicity of the elements and particularly on the notion of the tetra-atomicity of carbon, is that of the identical chemical function of the four valences of the carbon atom, which is not possible unless there exists only one methyl chloride, one methyl alcohol, etc. ... As for the three $C_2H_4Br_2$ isomers, given that they really exist, they are easily explained without having to assume a difference between the four affinities of the carbon atom, ..., when the four valences of the atom of this element are assumed to be arranged in the sense of the four angles of a regular tetrahedron. Then the first modification would have the two bromine atoms (or any other monovalent group) connected to the same carbon atom; while in the other modifications each of the two bromine atoms would be bonded to a different carbon atom, with only the difference that in one of the two cases the two bromine atoms would be arranged symmetrically but not in the other.

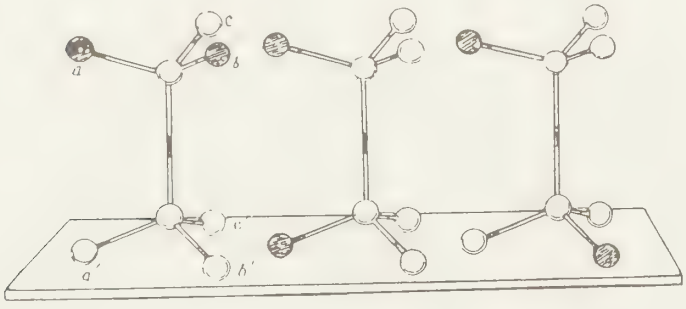


Figure 5. Illustration from Paterno's 1869 paper [*19*].

This is made clearer with the drawings in Figure 5 in which the bromine atoms are represented by a and b.

It was not, of course, until more than 70 years later that Odd Hassel published his conformational analyses of cyclohexane and derivatives by gas-phase electron diffraction [*21*].

Of the 20th century's development of structural chemistry, we mention the discovery of the electron-pair covalent bond by Lewis [*22*] which remains a fundamental tenet. It is remembered in every line we have drawn to represent a linkage and is present in most models of molecular structure, such as, for example, the valence shell electron pair repulsion (VSEPR) model [*23*].

IV. COMPARISON OF STRUCTURES

Comparison of structures has always been a rich source of information to account for and predict chemical behavior. This is because the chemical variation between molecules often reveals itself in the details of their geometry. Recently, Murray-Rust [*24*] noted the importance of comparative approach. He estimated that Linus Pauling [*25*] had access to less than 0.01% of the structural information of the early 1990s when he was writing the first edition of *The Nature of the Chemical Bond* in the late 1930s. Yet his ideas on structure and bonding have stood the test of time.

The seemingly obvious question of how similar is one molecule to another and one structure to another is far from trivial to answer. This has also been discussed recently by Murray-Rust [*24*]. Especially interesting are the multivariate statistical techniques enabling us to look for patterns and clusters in the structural data. Data banks are of great use. They include the Cambridge Structural Database at the University of Cambridge, the Inorganic Crystal Structure Database at the University of Bonn, and the Protein Data Bank at the Brookhaven National Laboratories (see e.g., [*24,26*]). For gas-phase molecular geometries, three volumes in the Landolt–Börnstein series constitute the data bank containing information on 2900 molecules through 1990 [*27*].

A. Representations

Today there is an arsenal of experimental physical techniques and computational methods for the determination of molecular geometry [*28*]. The respective precisions are often better than the various operational effects influencing these parameters, such as the consequences of the specificities of the matter/irradiation interaction and of molecular vibrations.

Different physical techniques utilize matter/irradiation events of different nature and may yield different features of the same structure. A schematic but pointed illustration of the problem is depicted in Figure 6 after Grimmer [*29*]. There are also different averaging procedures over molecular vibrations influencing the determined parameters. The first exposure of this problem was done by Bartell [*30*]

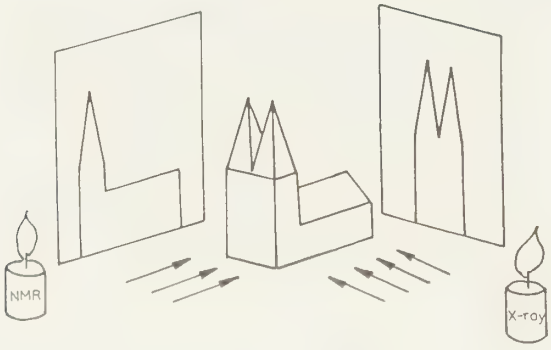


Figure 6. Grimmer's view of different features of the same object given by different experiments. Reprinted by permission of Kluwer Academic Publishers.

and it has been expanded and refined over the years with increasing accuracy requirements (see e.g., [*28*], and in particular, [*31*]).

The so-called operational parameters are the direct output of experimental studies. They do not have well-defined physical meaning. The most important and common ones are the following:

- r_a Effective internuclear distance, obtained directly from the analysis of electron diffraction intensities. Its conversion into r_g distance (see below) is simple with a very good approximation, $r_g \approx r_a + l^2/r_a$, where l is the mean vibrational amplitude. In other words, there is no need to use r_a in any comparison; it is preferable to use r_g.
- r_0 Effective internuclear distance, obtained from the rotational constants; usually refers to the ground vibrational state. Since it depends strongly on the isotopic composition, it may differ from the equilibrium distance by a couple of hundredths of an angstrom.
- r_s Effective internuclear distance determined from the isotopic substitution coordinates of the respective atoms. Since it depends slightly on the isotopic compositions, it may differ from the equilibrium distance by a few thousandths of an angstrom.

Internuclear distances with well-defined physical meaning are the following:

- r_e Equilibrium internuclear distance between equilibrium nuclear positions in the minimum position of the potential energy function. No experiment yields *directly* this parameter. All computed geometries, in principle, correspond to this distance, but only in principle, of course. Basis-set

Table 2. Factors Influencing Internuclear Distance Parameters

Distance Type	*Deformation Motion (e.g., bending, out-of-plane puckering)*	*Effect of Temperature*	*Effect of Isotope Composition*
r_g	+	+	+
r_α	–	+	+
r_α^0/r_z	–	–	+
r_e	–	–	

choice, approximations, and all computational conditions may influence the results.

r_g Distance-average incorporating the effect of all vibrations at temperature T. This is the parameter attainable in a straightforward way from electron diffraction.

r_α^0/r_z Distance between average nuclear positions in the ground vibrational state; r_α^0 and r_z have the same meaning; r_z originates from rotational spectra applying vibrational corrections. r_α is the distance between average nuclear positions averaged over all vibrational states at temperature T. r_α and r_α^0 are obtained from electron diffraction applying vibrational corrections.

The most unambiguous representation of molecular geometry is the r_e equilibrium structure. Another excellent representation of bond lengths is r_g since it is a real distance averaged over molecular vibrations. Distances r_α and r_α^0/r_z are less meritorious for characterizing bond lengths as they are projected averages, projected, that is, onto the direction of the lines connecting equilibrium nuclear positions. These representations are, however, the most suitable for characterizing bond angles. (On the other hand, a bond angle calculated from r_g distances has no well-defined meaning). A summary of effects of intramolecular motion on the various distance representations is given in Table 2.

B. Differences

The r_g/r_e differences increase with increasing floppiness of the molecule and with increasing experimental temperatures. However, these differences may extend beyond experimental error even for relatively rigid systems studied even at low temperatures. There are various ways to reduce the experimentally determined r_g distance to r_e distance, at least to a good approximation. A few examples are collected in Table 3 after Kuchitsu [*31*]. Recently Harmony [*12*] reviewed the possibilities of correcting spectroscopic information for vibrational effects, and made the following statement: "Finally after more than a half-century of spectro-

Table 3. Examples of r_g and r_e Bond Lengths[a,b]

	r_g(Å)	r_e(Å)	$\Delta(r)$(Å)	
C–H in CH_4	1.107(1)	1.0870 ± 0.0007	0.020	Rather floppy
B–F in BF_3	1.3133(10)	1.3070(1)	0.006	Rather rigid
C–O in Cl_2CO	1.184 ± 0.003	1.1766(22)	0.007	Rather rigid
C–Cl in Cl_2CO	1.744 ± 0.001	1.7365(12)	0.008	Rather rigid

Notes: [a]After Kuchitsu [*31*].

[b]Throughout this paper, the experimental errors are quoted in the following way: Least-squares standard deviations in parentheses as units of the last digit, e.g., 1.107(1) Å, and estimated total errors are quoted as error limits, e.g., 1.184 ± 0.003 Å

scopic structural studies, it now appears possible to obtain near-r_e bond lengths and angles for organic polyatomic molecules of modest size (6–8 heavy atoms)."

Careful considerations of the differences on the physical meaning of the parameters are needed as an increasing amount of experimental and computed structural information are being compared. As we stated: "For truly accurate comparison, experimental bond lengths should be compared with computed ones only following necessary corrections, bringing all information involved in the comparison to a common denominator" [*32*].

For floppy systems, such as many metal halide molecules, the r_g/r_e differences may be even much greater than those listed in Table 3. Alkaline earth metal, zinc, and transition metal dihalides, for example, have been extensively investigated by gas-phase electron diffraction (see e.g., [*33–36*]). The structure determinations have involved a joint electron diffraction/vibrational spectroscopic analysis (cf. [*37*]). Depending on the model potential used, and among them on the manner in which anharmonic effects are taken into account, even the "r_e" distances are rather different. This is illustrated by the data of Table 4. The r_e distances obtained from experimental data applying various model potentials [*32*] have the following

Table 4. Different Types of Bond Distances for Linear MX_2 Triatomic Molecules (in Å)[a,b]

MX_2	$ZnBr_2$	$MnCl_2$	$SrBr_2$
T(K)	600	1000	1400
r_g	2.204 ± 0.005	2.202 ± 0.004	2.783 ± 0.006
r_α	2.185 ± 0.008	2.162 ± 0.008	2.649 ± 0.024
r_e^h	2.181 ± 0.005	2.153 ± 0.005	—
r_e^{ch}	2.204 ± 0.004	2.196 ± 0.004	2.771 ± 0.006
r_e^a	2.196 ± 0.005	2.184 ± 0.005	—
r_e^M	2.196 ± 0.006	2.186 ± 0.005	2.738 ± 0.013

Notes: [a]References to the original publications: $ZnBr_2$ [*35*]; $MnCl_2$ [*36*]; $SrBr_2$ [*34*]

[b]See footnote [b] to Table 3

Table 5. Bond Distances for Bent MX_2 Triatomic Molecules (in Å)[a,b]

Molecule	*$SiCl_2$*	*$SiBr_2$*
T(K)	1470	1470
r_g	2.089 ± 0.004	2.249 ± 0.005
$r\alpha$	2.084 ± 0.004	2.244 ± 0.005
r_e^h	2.080 ± 0.004	2.239 ± 0.005
r_e^{ch}	2.081 ± 0.004	2.239 ± 0.004
r_e^a	2.076 ± 0.004	2.227 ± 0.006

Notes: [a]See footnote [b] to Table 3.
[b]From [*43,44*]

meaning: r_e^h harmonic approximation with rectilinear coordinates [*37*], r_e^{ch} harmonic approximation with curvilinear coordinates [*38*], r_e^a anharmonic approximation [*39*], and r_e^M distance with Morse-type anharmonic stretching correction [*40*]. The molecules listed in Table 4 have a linear equilibrium structure (except for $SrBr_2$ which is best labeled quasilinear [*34,41,42*]). Table 5 lists similar data for two

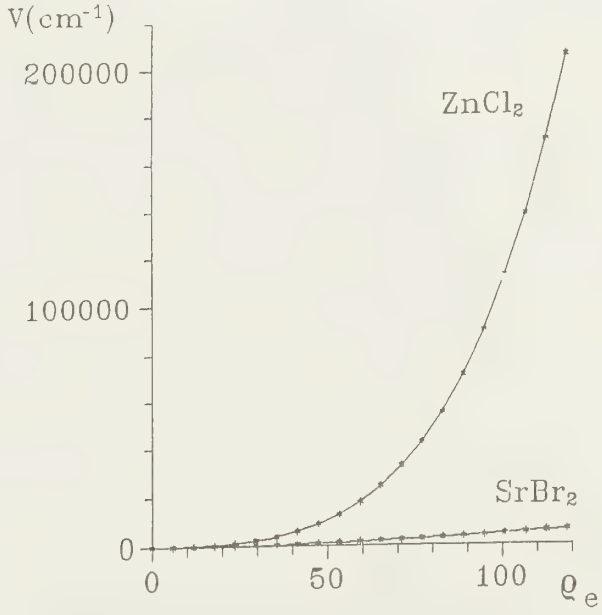


Figure 7a. Comparison of bending potential functions, linear models of $ZnCl_2$ and $SrBr_2$.

silicon dihalides which have a highly bent equilibrium configuration [*43,44*]. For all these systems it is especially important to define the type of distances that are being compared.

Any unambiguous determination of molecular geometry always includes considerations of motion. Its importance is illustrated here by the structure of three symmetric triatomic molecules involving linear, quasilinear, and bent ones [*45*]. The effective structure observed directly from the electron diffraction experimental data is invariably bent. The decisive difference appears in the shape of the potential energy function describing the bending motion. Examples are shown in Figure 7. The bending potential energy functions of $ZnCl_2$ and $SrBr_2$ are shown in Figure 7(a); $\rho_e = 0^\circ$ corresponds to the linear configuration. The minimum of potential

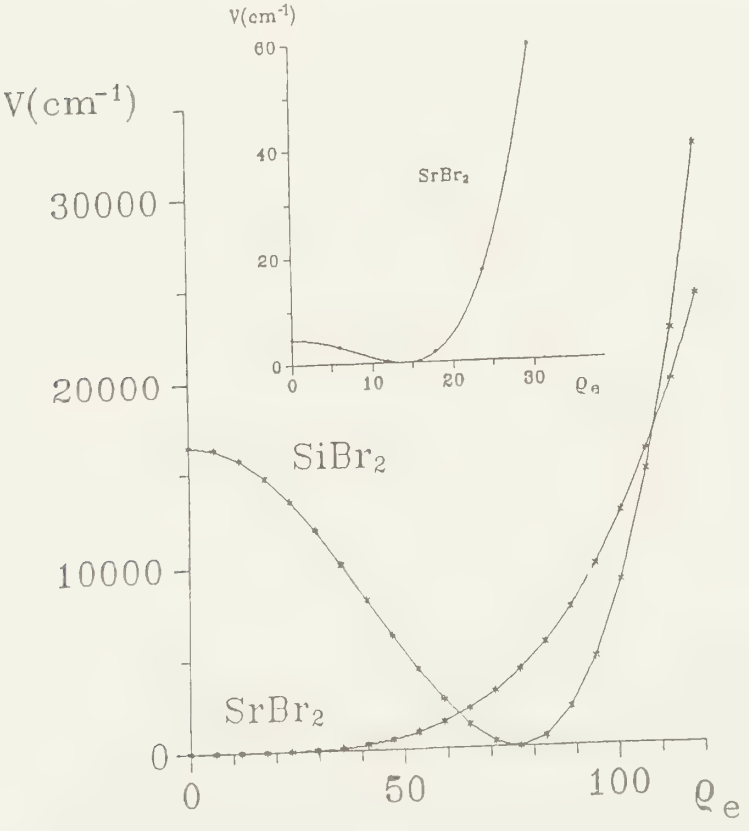


Figure 7b. Comparison of bending potential functions, bent models of $SrBr_2$ and $SiBr_2$.

energy appears to be at $\rho_e = 0^\circ$ for both molecules. It is also seen though that the minimum is much more shallow for $SrBr_2$ than for $ZnCl_2$. Figure 7(b) shows the bending potential energy functions of $SiBr_2$ and, again, $SrBr_2$. The relatively high barrier at $\rho_e = 0^\circ$ for $SiBr_2$ indicates an unambiguously bent configuration. Further enlarging the scale reveals a small barrier at $\rho_e = 0^\circ$ for $SrBr_2$, so small that it lies below the level of the ground vibrational state; hence the quasilinear designation for such a structure.

V. CHEMICAL SHAPE

Although the most unambiguous representation of molecular geometry is the equilibrium structure it may not always be the most useful one. Real molecules in real reactions spend very little time in or near their equilibrium structure, especially if they are characterized by large-amplitude vibrations. Levine [*46*] calls it the task of dynamical stereochemistry to determine the *chemical shape* of molecules. He suggests to distinguish the physical and chemical shapes, and finds that the interplay between the two accounts for much of the detail provided by experiments and computational studies. According to Levine [*46*], the chemical shape describes how molecular reactivity depends on the direction of approach and distance of the other reagent. On the other hand, the physical shape corresponds to a hard space-filling model.

The concept of chemical shape is important whenever any kind of interaction between molecules is involved. Thus, Levine's characterization of chemical shape is fully consistent with Legon's description of *molecular recognition* [*47*]:

> At the fundamental level, molecular recognition involves the specific interaction of one part of a molecule with a particular part of another molecule. This interaction will be defined by a relative orientation and by a separation of the two subunits that confer on the system as a whole a lower energy than other conformations. An understanding of the fundamentals of molecular recognition therefore requires a knowledge of the properties of intermolecular interactions and in particular how the energy varies with relative orientation and separation.

VI. INTRAMOLECULAR INTERACTIONS

Following the structural consequences of ligand substitution in series of substances has been a rewarding approach in investigating correlations between structure and bonding and other properties.

The S–C and Se–C bond lengths, for example, are sensitive to the valence state of the participating carbon [*48*] (Figure 8). The effects are large and the differences may exceed 0.1 Å. Ligand substitution on carbon causes appreciable, though lesser, bond-length changes in the sulfides and selenides. On the other hand, ligand substitution on carbon may cause changes again up to 0.1 Å in the S–C bond lengths in sulfones. Thus, for example, S–C changes from 1.763(5) to 1.865(6) Å upon CH_3/CF_3 substitution, from CH_3SO_2Cl [*49*] to CF_3SO_2Cl [*50*]. The difference is

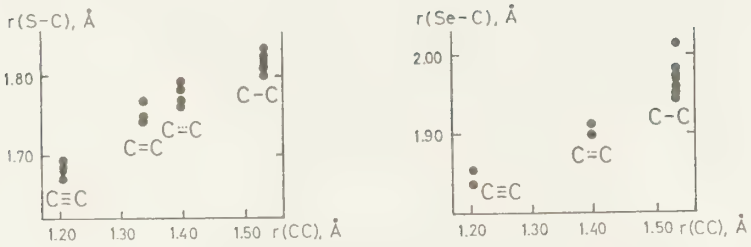
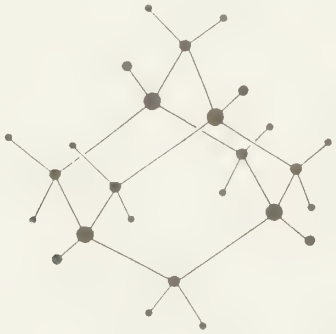


Figure 8. S–C and Se–C bond lengths in sulfides and selenides with various carbon valence states (after [*48*]).

interpreted as a consequence of the electron releasing ability of the methyl group and the electron withdrawing ability of the trifluoromethyl group.

There is a much smaller but still significant difference in the C–C bond lengths of adamantane, $C_{10}H_{16}$ [*51*], and perfluoroadamantane, $C_{10}F_{16}$ [*52*], depicted in Figure 9. The bond lengthening is thought to be a consequence of the electron-withdrawing ability of the fluorine ligand as compared with hydrogen.

Very weak interactions may also have appreciable geometrical consequences. An example is the structure of *N*,*N*-dimethyl-formamide [*53*] (Figure 10). There is a



	r_g(C–C)
$C_{10}H_{16}$	1.542±0.002 Å
$C_{10}F_{16}$	1.560±0.003 Å

Figure 9. C–C bond length of adamantane [*51*] and perfluoroadamantane [*52*].

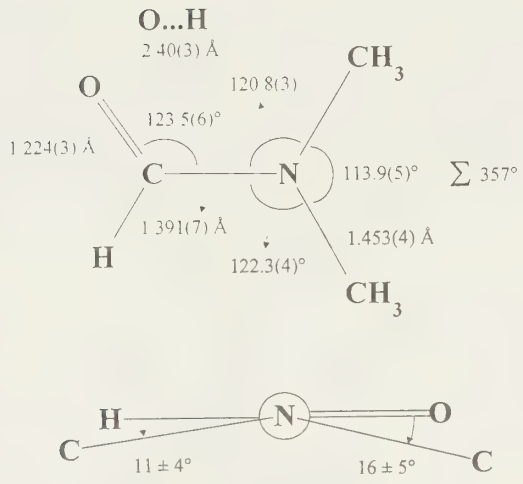


Figure 10. *N,N*-dimethylformamide structure from gas-phase electron diffraction [*53*].

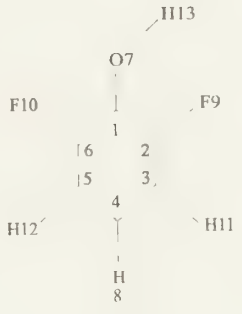
difference between the two (O)C–N–C angles. The one *syn* to the C=O bond is somewhat smaller than the other. The C=O...H–C nonbonded distance, 2.40 ± 0.03 Å, indicates some attractive interaction, although it is far too long to consider it a hydrogen bond. Comparison with formamide [*54*] itself, which cannot have an O···H interaction, supports the notion of the presence of some attractive interaction in the *N,N*-dimethyl derivative. Formamide has a somewhat shorter C=O bond, 1.212(2) Å, and a somewhat greater N–C=O angle, 125.0(4)°, than *N,N*-dimethylformamide. The O···H nonbonded interactions are manifested in yet shorter O...H distances in *N,N*-dimethylacetamide (2.21 Å) and *N*-methylacetamide (2.33 Å) according to recent high-level *ab initio* calculations [*55,56*] (the O···H distances given here were calculated from the published geometries of refs. [*55*] and [*56*], respectively).

In Section IV.B, we have stressed the importance of the physical meaning of parameters in a demanding comparison. There are other situations where trends and patterns in the parameters and their changes are sought. This can be done even without corrections for vibrational effects or other conversions. This is especially so when looking for patterns in data collected by the same technique in the same laboratory. Table 6 presents some geometrical parameters of 2-fluorophenol [*57*], 2,6-difluorophenol [*58*], and tetrafluorohydroquinone [*58*]. There are several geometrical features that can be ascribed to the consequences of some weak hydrogen-bond formation. They also seem to indicate a trend according to which the hydrogen bonds may strengthen from 2-fluorophenol toward tetrafluorohydroquinone. On

Table 6. Selected Geometrical Parameters of 2-Fluorophenol, 2,6-Difluorophenol, and Tetrafluorohydroquinone[a]

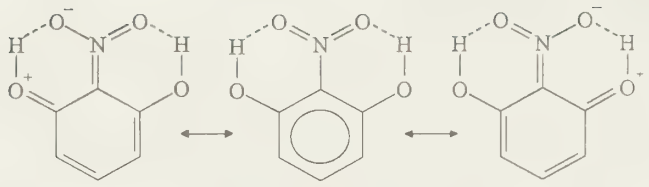
	2-Fluorophenol[b]	*2,6-Difluorophenol*[c]	*Tetrafluorohydroquinone*[d]
$H_{13}\cdots F_9$, Å	2.125 ± 0.055	2.054 ± 0.079	2.015 ± 0.069
$O_7\cdots F_9$, Å	2.735 ± 0.022	2.715 ± 0.067	2.657 ± 0.054
∠C–O–H, deg	101.9 ± 3.9	96.7 ± 4.2	98.2 ± 2.4
$r(C_2–F_9)$, Å	1.353 ± 0.012	1.358 ± 0.056	1.350 ± 0.012
$r(C_6–F_{10})$, Å	—	1.346 ± 0.048	1.343 ± 0.013
$\angle C_3–C_2–F_9$, deg	120.3 ± 4.8	120.1 ± 2.3	122.1 ± 1.7
$\angle C_5–C_6–F_{10}$, deg	—	118.5 ± 3.8	119.6 ± 0.9
tilt, deg	− 0.7 ± 4.0	0 (assumed)	2.1 ± 1.2
$r(C_1–O_7)$, Å	1.378 ± 0.010	1.362 ± 0.036	1.353 ± 0.009
$\angle O_7–H_{13}\cdots F_9$, deg	120.8 ± 4.5	127.1 ± 5.1	123.8 ± 2.9
$\angle C_2–F_9\cdots H_{13}$, deg	79.0 ± 1.7	77.7 ± 3.3	80.2 ± 1.6
R	0.0280	0.0281	0.0269

Notes: [a]Distances are r_g values.
[b]Ref. [57]
[c]Ref. [58]
[d]Ref. [57].

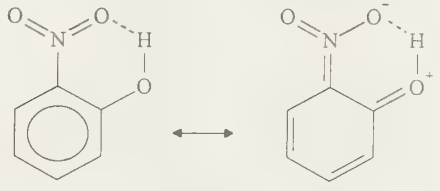


the other hand, no geometrical indication pointing to hydrogen bonding was detected in 2,6-difluorobenzenamine and 2-fluorobenzenamine [*59*].

Relatively strong intramolecular hydrogen bonding was indicated by the geometry of 2-nitroresorcinol [*60*] and 2-nitrophenol [*61*] from gas-phase electron diffraction studies. There are considerable bond-length changes in these molecules as compared with nitrobenzene [*62*] and phenol [*63*]. These changes are consistent with strong resonance-assisted hydrogen bonding. Such resonance-assisted hydrogen bonding has been described for a number of crystal molecular structures [*64*]. Schemes 1 and 2 show the resonance forms of 2-nitroresorcinol and 2-nitrophenol that are supposed to contribute strongly to the molecular structure. The experimental evidence is unambiguous for the longer N=O bonds and shorter N–C bond in 2-nitroresorcinol than in nitrobenzene, and for the shorter C–O bonds and longer O–H bonds than in phenol. The experimental geometries are characterized in Table 7. Differences in the geometrical parameters are collected in Table 8. Along with



Scheme 1.



Scheme 2.

Table 7. Geometrical Parameters of Phenol, Nitrobenzene, 2-Nitrophenol, and 2-Nitroresorcinol from Gas-Phase Electron Diffraction[a]

Parameter	*Phenol*[b]	*Nitrobenzene*[c]	*2-Nitrophenol*[d]	*2-Nitroresorcinol*[c]
C_1–C_2, Å		1.400(3)	1.411(12)	1.426(5)
C_2–C_3, Å	1.399(3)		1.406(13)	
C_3–C_4, Å		1.396(3)	1.388(21)	1.393(4)
N=O_{14}, Å	—	1.223(3)	1.241(9)	1.239(3)
N=O_{15}, Å	—		1.225(9)	
C–N, Å	—	1.486(4)	1.464(5)	1.449(7)
C–O, Å	1.381(4)	—	1.359(9)	1.354(4)
O–H, A	0.958(3)	—	0.969(12)	1.038(15)
∠C–N=O_{14}, deg	—	117.3(1)	118.2(10)	119.3(3)
∠C–N=O_{15}, deg	—		118.6(10)	
∠O=N=O, deg	—	125.3(2)	123.3(4)	121.4(5)
∠C–O–H, deg	106.4(17)	—	104.4(22)	116(3)
∠N–C_1–C_2, deg	—	117.4(2)	120.8(7)	120.5(4)
∠O–C_2–C_1, deg	121.2(12)	—	123.9(8)	122.8(7)
∠C–C_1–C, deg	121.6(2)	123.4(3)	121.4(5)	119.1(7)
∠C–C_2–C, deg	118.8(2)	117.7(3)	119.4(8)	120.4(5)
CO, tilt, deg	+2(1)	—	+3.6(7)	+2.9(5)
(N=)O···H(–O), Å	—	—	1.72(2)	1.76(4)
(N=)O···O(–H), Å	—	—	2.58(1)	2.56(1)
∠N=O···H, deg	—	—	104.3(15)	110.5(15)
∠O–H···O, deg	—	—	147(3)	131(5)

Notes: [a]Distances (r_g bond lengths) in Å, angles in degrees.
[b]Ref. 63.
[c]Ref. 62.
[d]From a concerted analysis incorporating constraints from MP2(FC)/6-31G* *ab initio* calculations, ref. 61.
[e]Ref. 60

the experimental data, the differences referring to quantum chemically calculated parameters are also given [*61*,*65*]. Emphasis is on the comparison of differences which are free of a variety of problems that the absolute values of both the experimental and calculated results may suffer from.

Of 2-nitroresorcinol and 2-nitrophenol, the former has higher symmetry and is an easier target for gas-phase electron diffraction. On the other hand, the structure of 2-nitrophenol could not have been determined without the introduction of some constraints from quantum chemical calculations. These constraints, however, have always meant differences between parameters rather than actual bond lengths or bond angles. Heretofore, we have mentioned the geometrical consequences of the strong hydrogen-bond formation in 2-nitroresorcinol and 2-nitrophenol. Tables 7 and 8 list the O···H (N=O···H–O) and O···O (N=O···O–C) nonbonded distances that can be considered direct evidence of the strong hydrogen bonds. Usually such distances, and especially the O…H distance, can be inferred only indirectly in an electron diffraction study because of their small relative weight among interactions in the electron scattering process. Figure 11 shows that, by a rare favorable coincidence, there is a broad valley in the vicinity of the contribution of the O···H distance on the radial distribution of 2-nitroresorcinol. The radial distribution is an expression of the probability density distribution of the internuclear distances obtainable from the electron diffraction data [*66*]. In this case, a distinct feature, however slight, can be ascribed to the contribution of the O···H distances in the

Table 8. Differences of Selected Parameters[a] Demonstrating Geometrical Consequences of Intramolecular Hydrogen-Bond Formation

	2-Nitrophenol/Phenol		*2-Nitroresorcinol/Phenol*	
Parameter	*Electron Diffraction*	*Calculation MP2(FC)/6-31G**	*Electron Diffraction*	*Calculation MP2(FC)/6-31G**
O–C, Å	– 0.022	– 0.024	– 0.027	– 0.024
(O)C–C(N), Å	+ 0.012	+ 0.014	+ 0.027	+ 0.028
O–C–C(N), deg	+ 2.7	+ 2.8	+ 1.6	+ 1.9
CO tilt, deg	+ 1.6	+ 1.3	+ 1	+ 1.2
	2-Nitrophenol/Nitrobenzene		*2-Nitroresorcinol/Nitrobenzene*	
Parameter	*Electron Diffraction*	*Calculation MP2(FC)/6-31G**	*Electron Diffraction*	*Calculation MP2(FC)/6-31G**
N–C, Å	– 0.022	– 0.015	– 0.037	– 0.032
(O)C–C(N), Å	+ 0.011	+ 0.018	+ 0.026	+ 0.033
N–C–C(O), deg	+ 2.5	+ 2.4	+ 3.1	+ 2.6
O–N–C(O), deg	+ 0.9	+ 0.7	+ 2.0	+ 2.0
CN tilt, deg	+ 1.5	+ 1.8	—	—

Note: [a]For references, see text.

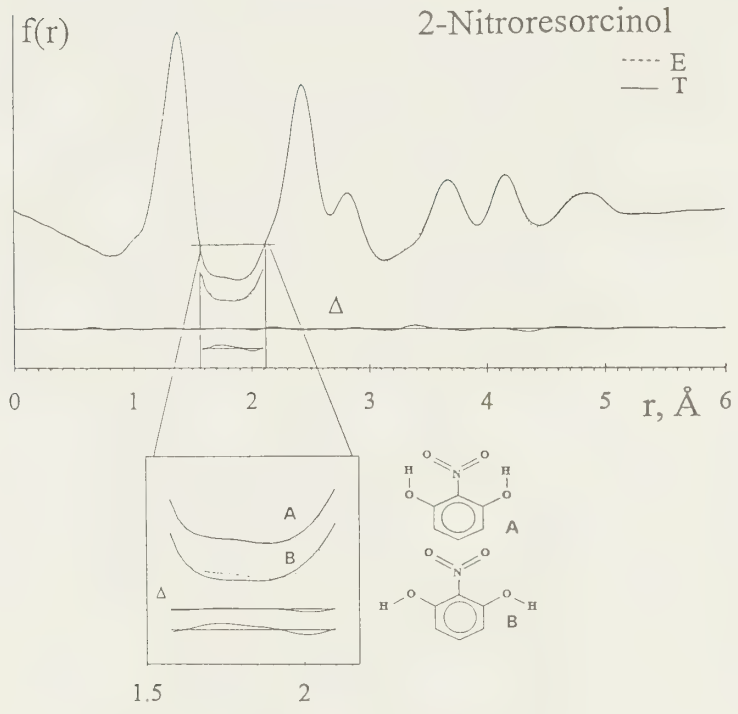
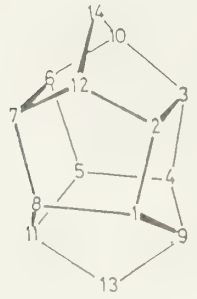


Figure 11. 2-nitroresorcinol: radial distributions [*60*].

structure with the hydrogen bonds. This is made clear by the comparison with the curve calculated for another form in which there is no such hydrogen bond.

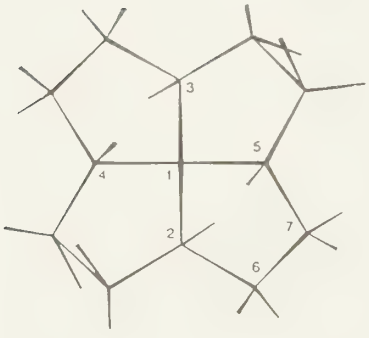
Another example of geometrical consequences of intramolecular interactions can be demonstrated by the structure of a few carbon-cage molecules. Whereas the adamantane molecule [*51*] has only one kind of C–C distance, due to its high symmetry, there is a distribution of C–C distances in, for example, heptacyclotetradecane (Figure 12(a)) [*67*] and fenestrane (Figure 12(b)) [*68*] due to intramolecular nonbonded interactions.

A final example of intramolecular interactions concerns the geometrical changes upon internal rotation. In a variety of situations, such as, e.g., conformational equilibria in the gas phase or structures of the same molecule in different phases, such effects may be of importance. Thus, for example, the C–C–X bond angles of 1,2-dihaloethanes were calculated to change up to 4° during internal rotation [*69*]. Ignoring this change may cause an error up to 11° in the determination of the gauche angle of torsion for a mixture of *anti* and *gauche* conformers.

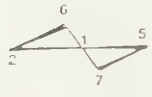


(a)

r_g C_1–C_8 1.586±0.004 Å
C_1–C_2 1.528±0.006 Å
C_1–C_9 1.553±0.004 Å
C_9–C_{13} 1.532±0.004 Å



r_g C_1–C_2 1.558±0.005 Å
C_2–C_6 1.539±0.008 Å
C_6–C_7 1.542±0.013 Å
$<C_2$–C_1–C_3 116.2±0.5°
$<C_2$–C_1–C_5 106.2±0.2°



(b)

Figure 12. (a) C–C bond lengths of heptacyclotetradecane [*67*]. (b) C–C bond lengths of fenestrane [*68*].

VII. INTERMOLECULAR INTERACTIONS

Until some time ago, crystallographers used to assume that the molecules have the same structure in the crystal as the free molecules in the vapor (see, e.g., [*70*]). With increasing capabilities of structure determination the gas/crystal structure differences are gaining importance. Their elucidation is rapidly becoming a most important source of information on the intermolecular interactions in the crystal (see, e.g., [*71–73*]). The origin of gas-phase structures is not only the experimental techniques, such as electron diffraction and high-resolution rotational spectroscopy but, increasingly, high-level *ab initio* molecular orbital calculations. The result of the latter also refer to the free molecule.

Again, as with any comparison of structural information, first all operational effects must be eliminated before any difference is to be ascribed to truly structural effects. Thus, for example, further corrections are necessary before making conclusions from a comparison of r_g electron diffraction and r_α X-ray diffraction bond lengths. The true r_α parameter refers to distances between average nuclear positions. As is well known, X-ray diffraction provides distances between the centroids of the electron density distribution rather than internuclear distances. However, for spherically symmetrical electron density distributions, coincidence with the nuclear positions can be assumed. Thus following corrections for the so-called asphericity effects (as well as for rigid-body librations), the X-ray results can be considered as an r_α structure. Thus, especially for bond angles, the comparison may provide meaningful information.

Considering the energy requirements of structural changes and the energy contents of crystal-field effects, conformational changes, angular changes, and bond length changes may be expected in diminishing order. It has been estimated [*72*] for a carbon–carbon chain that a typical bond stretching of 0.1 Å requires about 15 kJ/mol, a bond-angle deformation of 10°, about 5 kJ/mol, and a torsional distorsion of 15°, about 1 kJ/mol. However, as was mentioned at the end of the previous section, these changes (e.g., torsion and angle bending) do not occur separately but should be considered as parts of the overall structure relaxation and treated in a concerted way, especially beyond certain accuracy requirements.

There are now at least a few well-documented cases of gas/solid structure differences involving the consequences of intermolecular hydrogen bonding and other interactions in the crystal. In addition to gas/solid comparison, comparison of crystallographically independent molecules in the same crystal, analysis of the structure of molecules whose symmetry is lower in the crystal than in the vapor, and comparison of molecular structures in different polymorphic modifications are the principal venues to investigate the influence of intermolecular interactions on molecular structure. These strategies were identified by Kitaigorodskii [*74*] at a very early stage of accurate crystallographic studies. It was yet another example of the prescience of this great crystallographer, and especially so since previously he had dismissed the possibility of appreciable gas/solid structural changes. Incidentally, a memorial collection of papers with the title, *Molecular Crystal Chemistry*, was recently published as an homage to him [*75*].

The understanding of changes in molecular structures is important not only in the investigation of intermolecular interactions in crystals. Another area is the investigation of large and often biologically important systems. Considerations of the chemical shape, molecular recognition, and the energy costs of changes converge. According to Legon [*47*]:

> For the purpose of modeling large systems, it is of interest to follow an approach familiar in chemistry, i.e., to consider the larger systems to be composed of groups, each group having its own characteristic properties. Thus, we might enquire into the preferred angular and radial

geometry for the interaction of one group with another and, given that in a larger unit it might not be possible to achieve the preferred arrangement, we might then ask about the cost in energy of small angular and radial distortions for this conformation.

As a final note in this section we mention a recent attempt to establish some correlation between gaseous molecular structures and their source crystal structures of highly ionic substances [*76*]. For some metal halides both monomers and dimers occur in the vapor phase, while for others only the monomer is present in appreciable amounts. Systematic comparisons reveal that dimers are not detected in the vapor if the dimeric molecule cannot be recognized as a unit in the crystal structure. On the other hand, if the presence of dimeric molecules is discernible already in the crystal, it will be observed in the vapor only if its heat of vaporization does not exceed that of the monomer by more than, say, 10 kcal/mol.

VIII. CRYSTAL ENGINEERING

Different changes in the molecular structure of analogous compounds observed in gas/crystal comparisons reflect differences in molecular packing. An example is the different impact on the benzene ring deformation by intermolecular interactions in the crystals of *p*-dicyanobenzene [*77*] and *p*-diisocyanobenzene [*78*] as illustrated in Figure 13. There is a network of dipole–dipole interactions between the antiparallel cyano groups in the crystal of *p*-dicyanobenzene. The packing of *p*-diisocyanobenzene molecules, on the other hand, allows charge-transfer interactions.

The understanding of crystal packing in terms of intermolecular interactions and using this understanding to design crystals with perceived packing and properties is the subject of crystal engineering [*79*]. It also follows from the foregoing that the understanding of relatively weak interactions and their geometrical consequences in molecular structure is one of the determining factors in crystal engineering. Intermolecular hydrogen bonding is perhaps the single most important one among the possible weak interactions. It has been called to be the most dominant mechanism of molecular recognition in crystals [*80*]. Also, intermolecular hydrogen bonds may not be so weak, especially when acting in large numbers. Their cooperative action was nicely illustrated by Jeffrey and Saenger [*81*] who showed Gulliver, the giant, constrained by a multitude of weak bonds (Figure 14).

With all the progress, however, it is still difficult to predict crystal structures. This frustration was powerfully expressed by Maddox [*82*]: "One of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition." There is also considerable progress during the past few years in this respect, mainly due to the utilization of the wealth of information retrievable from the data banks, and especially the Cambridge files [*83*].

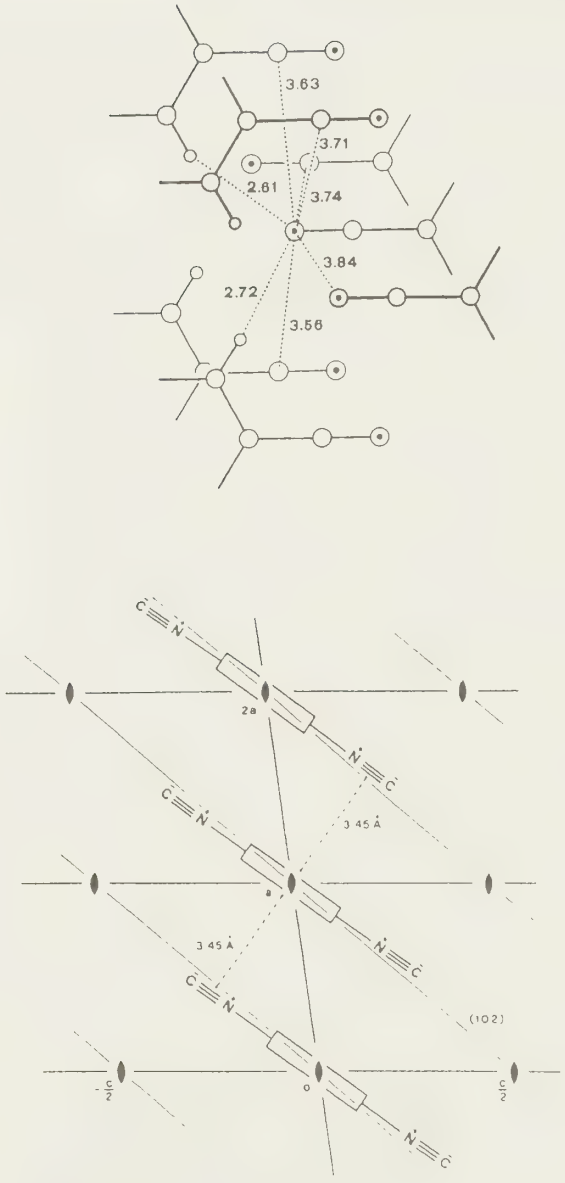


Figure 13. Arrangements of molecules in crystalline *p*-dicyanobenzene [*77*] and *p*-diisocyanobenzene [*78*] demonstrating a marked difference in packing (see text).

Figure 14. After Jeffrey and Saenger's [*81*] idea to illustrate cooperative action: Gulliver: a giant, constrained by a multitude of weak bonds. Illustration by V. Kubasta in J. Swift, Gulliver Lilliputban, © Artia, Praha.

The design of drugs and extremely strong and long-lasting materials are two conspicuously important domains of crystal engineering. The determination of structures, the elucidation of structure/activity correlations involving advanced computational techniques allow the design of desired drugs based on stereochemical principles. Yet the elimination of some illnesses may necessitate not only drugs but the solution of social and environmental problems [*84*]. Concerning the design of new materials, environmental concerns have enhanced the requirements against which their applicability can be measured [*85*].

IX. SUPRAMOLECULAR STRUCTURES

A molecular crystal is a result of molecular self-assembly but it is not the only example of such molecular organizations. The living organism has ranges of self-assembled structures [*86*]. Needless to say, structural information from the simplest molecules to those with increasing complexity are decisive in designing and understanding such molecular self-assemblies. Whereas two-dimensional and three-dimensional networks have previously been of primary interest to the inorganic chemist (see, e.g., Wells [*87*]), this has recently become a focal point in organic chemistry as well [*88*]. Again, there is emphasis on weak interactions of a great variety. According to Lehn [*89*]: "Beyond molecular chemistry based on the covalent bond lies supramolecular chemistry based on molecular interactions—the associations of two or more chemical entities and the intermolecular bond." There is then a complete analogy between the atoms linked by covalent bonds into molecules and the molecules linked by intermolecular interactions into supermolecules [*90*]. Lehn has also established a linkage between molecular and supramolecular chemistries through molecular recognition when he stated succinctly [*91*] that "molecular recognition implies the (molecular) storage and (supramolecular) retrieval of molecular structural information." The investigation of these molecular and supramolecular systems represent true challenges for structural chemistry.

NOTE

1. Latin. In English: "Where there is matter, there is geometry"

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FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

January 24, 1996

TO: Professor Istvan Hargittai
Budapest Technical University
FAX: 36-1-465-4052

Dear Istvan:

The January *Chemical Intelligencer* arrived at home yesterday, and I spent a delightful evening reading it from cover to cover.

Do you need any more information to include the Loschmidt stamp in one of your next issues?

I note that my Parsons Award address on chemophobia will be included in your April issue. And in such good company: Both Pierre Laszlo and Derek Davenport are old friends who have also published essays in the *Aldrichimica Acta*. I particularly look forward to Derek's article on oprobium with - I am sure - very useful advice. At least useful to characters like myself!

Will you also include Bruce Buchan's paper?

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

Yours sincerely,

AB/cw

FOR: ALFRED HARER FINE ARTS

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GALLEY PROOFS FOR YOUR CONTRIBUTION TO THE CHEMICAL INTELLIGENCER

Attached please find the galley proofs of your contribution to The Chemical Intelligencer, which is scheduled for publication very shortly.

In order to ensure prompt corrections, it is imperative that you read the proofs for typographical or stylistic errors and that you return proofs to the The Chemical Intelligencer editor within 48 hours of receipt. Please either fax (if corrections are few) or send by **overnight courier** to:

Dr. Istvan Hargittai
Budapest Technical University
SZT. Gellert ter 4
H-1111 Budapest, XI.
HUNGARY

Fax: (36-1) 463-4052

Although the corrections are made immediately, the article is not necessarily scheduled for the next next issue. It may be scheduled for a future issue, but we find it best to make the corrections at this time.

If there are any questions, call Dr. Hargittai at (36-1) 463-4051 or send e-mail: hargittai@ch.bme.hu.

Only the Copyright/Offprint form **must be returned to me** at Springer-Verlag.

Thank you for your cooperation in this matter.

Sincerely,

Madeline R Kraner

Madeline R. Kraner
Assistant Manager, Magazine Production

FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

February 6, 1996

TO: Professor Istvan Hargittai
Budapest Technical University
FAX: 36-1-463-4052

Dear Istvan:

Thank you so much for your letter.

Of course, the Parsons Award address could be published in the *Chemical Intelligencer* anytime.

When you were here, we discussed the Josef Loschmidt stamp published by the Austrian post office last summer, and I gave you the details of the stamp. You have such an interesting stamp corner, and I thought that a discussion of the stamp by your expert on stamps would be interesting.

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

Yours sincerely,

AB/cw

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FAX FROM

DR. ALFRED BADER
Suite 622
924 East Juneau Avenue
Milwaukee, Wisconsin 53202
Telephone: 414/277-0730
Fax: 414/277-0709

February 7, 1996

TO: Professor Istvan Hargittai
Budapest Technical University
FAX: 36-1-463-4052

Dear Istvan:

I have just received the FedEx package from Ms. Madeline Kraner at Springer in New York including the Chemophobia galleys, and three pages of the final article.

However, page three ends with the line "Aldrich without the good chemists there, so" and four lines of the article are missing. Could you perhaps fax me those four lines?

Looking over the article, it looks excellent, with just a few commas missing. Also, many of the titles, such as *Adventures of a Chemist Collector*, are not in italics. I will fax you the corrected copy no later than tomorrow afternoon.

You may recall that I told you during your visit that I had given Professor Zdenek Herman in Prague permission to translate the article into Czech and then to have it published in a Czech chemical journal. Hence, I have deleted "and translations" from the copyright transfer statement, which I am mailing to Ms. Kraner.

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

AB/cw

cc: Madeline R. Kraner (by fax)

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September 6, 1995

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

Dear Dr. Bader:

Enclosed is a complimentary copy of our new book *Symmetry*, by István & Magdolna Hargittai. It has been two years in the making, and is, we feel, unique in several respects:

1. It is the first comprehensive book on a subject that has fascinated people for millenia.
2. It is written in clear, non-technical language. Our aim was that a high school student would be able to understand the text.
3. It is highly visual and in fact, a great deal about the subject can be learned by just looking at the photos and reading the captions.
4. It has as an underlying theme: the unification of diverse fields of knowledge via the subject of symmetry.

We would be most interested in your reaction to *Symmetry.* If you are so inclined, we would appreciate a written comment—a sentence or two would suffice. We intend to use such comments to publicize the book.

Or, if you are in a position to review the book, please do so. Also, if you can think of any publication we might send a copy to, please give us the name and address and we will send a book; this could be anyone who might review *Symmetry*, or anyone in a position to inform the public about the book. The book does not really fit into any category, so we think that word-of-mouth will, in the long run, be a good source of publicity.

The authors are two internationally known structural chemists from Budapest. It is their aim and hope that after looking through *Symmetry,* the reader will then see new patterns and make new connections in the visible world. We have already found this to be true with people who have seen advance copies of the book. (Our German agent said that when she and her daughter visited the Grand Canyon, "We saw symmetries everywhere.") We hope this happens with you too!

Yours sincerely,

Lloyd Kahn
Editor

". . . the cumulative effect of the book is to create the feeling in the reader that all life is visual art and that most of it has some relationship to symmetry—exactly what the authors are trying to suggest. A unique look at life and creation."

-Brian McCombie
Booklist

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

A Chemist Helping Chemists

November 13, 1995

Professor Istvan and Dr. Magdalena Hargittai
c/o Budapest Technical University
Budapest, XI. SST.
Gellért tér 4. H-1521
Hungary

Dear Magdalena and Istvan:

It was such a pleasure to be able to meet you personally last week, and I want to thank you most sincerely for all the time which you spent with us. We already look forward to your next visit.

I am asking one of my best friends at Aldrich to put you, Istvan, onto the *Aldrichimica Acta* mailing list. I presume that one copy will suffice.

As you know, we are just leaving for England, but soon after my return to Milwaukee on December 24th, I will get together a set of the *Actas*, including the very latest, and send these to you for your personal library.

With all good wishes, I remain,

Yours sincerely,

AB/cw

P.S.

My excellent British literary agent is Jeffrey Simmons, whose address is 10 Lowndes Square, London SW1X 9HA, England; Ph: 44-171-235-8852 and Fax: 44-171-235-9733.

P.S. to Delores:

Thank you so much for your long fax, which I appreciate more than I can tell you.

Professor Istvan Hargittai is a brilliant chemist in Budapest, and his wife is a well-known researcher at the Academy of Sciences. Could you please put Professor Istvan Hargittai onto the *Aldrichimica Acta* mailing list?

I think I have planted the seed in his mind to look for Sigma-Aldrich Library chemicals collections in Budapest.

With all good wishes, as always,

AB/cw

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

A Chemist Helping Chemists

November 8, 1995

Via hand delivery at Astor Hotel

Professor Dr. Istvan Hargittai
c/o Astor Hotel

Dear Professor Hargittai:

Welcome to Milwaukee. I hope that you and Mrs. Hargittai will find this hotel comfortable.

A professor of business at Queen's University has looked at your new publication, *The Chemical Intelligencer*, carefully and has asked me to submit a paper for your consideration. Two copies of that are enclosed.

If you would like to discuss this with Professor Buchan, we could call him from my office tomorrow.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Enclosures

FAX FROM:

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

A Chemist Helping Chemists

November 1, 1995

TO: Professor Dr. Istvan Hargittai
~~Professor of Chemistry~~
Budapest Technical University
FAX: ~~36-1-463-4052~~

Dear Professor Dr. Hargittai:

I am sorry that a trip to Canada has delayed my responding to your fax of October 28th.

I enclose details about how to get to my office.

The drive from downtown Chicago to my office takes about 2 hours. If you would like, we could make a hotel reservation, guaranteed for late arrival, at the Astor Hotel, where my gallery is. It is an old-fashioned, clean hotel.

If you should come to the hotel on Thursday morning rather than on Wednesday evening, please just drive into the parking lot north of the hotel and tell the attendant that you are visiting Alfred Bader. That way you avoid the parking charge.

I get to my office around 8:00 am and of course hope that both of you will be able to join me for lunch after our discussions.

With all good wishes, I remain,

Yours sincerely,

AB/cw

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

A Chemist Helping Chemists

I-94 to the Bader Gallery

Coming from Chicago, take I-94 north.

When you come close to downtown, take the exit marked East 794. (The exit before is National Avenue; do not take National.)

On 794, go east close to Lake Michigan and take the exit marked Jackson & Van Buren.

Take Van Buren north (approximately 8 blocks) to Juneau Avenue.

There, turn right for three (3) blocks to the Astor Hotel at 924 East Juneau Avenue.

The parking lot for the hotel is north of the hotel.

FOR: ALFRED BADER

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RECEIVER	[illegible]	[illegible]
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BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4051, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred B[illegible]
2961 North Shephard Avenue
Milwaukee WI 53211

Dear Dr. Bader [illegible]

We are departing for the U.S. Thursday morning, November 2. At this time I would like to finalize the details of our visit to you in the morning of Thursday, November 9. The previous afternoon we'll be driving from West Lafayette to Milwaukee, and will be staying overnight most probably in a motel somewhere between Chicago and Milwaukee. I don't think that this will be far from the center of Milwaukee and we don't mind getting up early, so we could come to see you right in the morning.

I would appreciate getting directions how to find you. Please, don't mind giving details that may seem trivial to you. We have never been to Milwaukee and I am not a [illegible]

Both my wife and I have read your book and are taking with us to study it more during [illegible]

We are looking forward to seeing you soon, but, of course, first to hearing from you [illegible]

[illegible]

István Hargittai

Dr. Alfred Bader
2961 North Shephard Avenue
Milwaukee, WI 53211

The Chemical Intelligencer

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e-mail: hargittai@ch.bme.hu
tel: (36-1) 463-4051
fax: (36-1) 463-4052

September 6, 1995

Dear Dr. Bader:

This is a sequel to my letter of September 3 to you. At that time I was so overwhelmed by your book that I forgot the most obvious thing: I am cordially inviting you to write for *The Chemical Intelligencer*. You may consider anything from brief notes to full articles.

I often think of various things that I'd read in your book. I also feel that you may very well have more to say.

With kind regards,

Sincerely,

Istvan Hargittai

FAX FROM:

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

A Chemist Helping Chemists

August 29, 1995

Via Facsimile: 36-1-463-4052

TO: Professor Dr. István Hargittai
Professor of Chemistry
Budapest Technical University

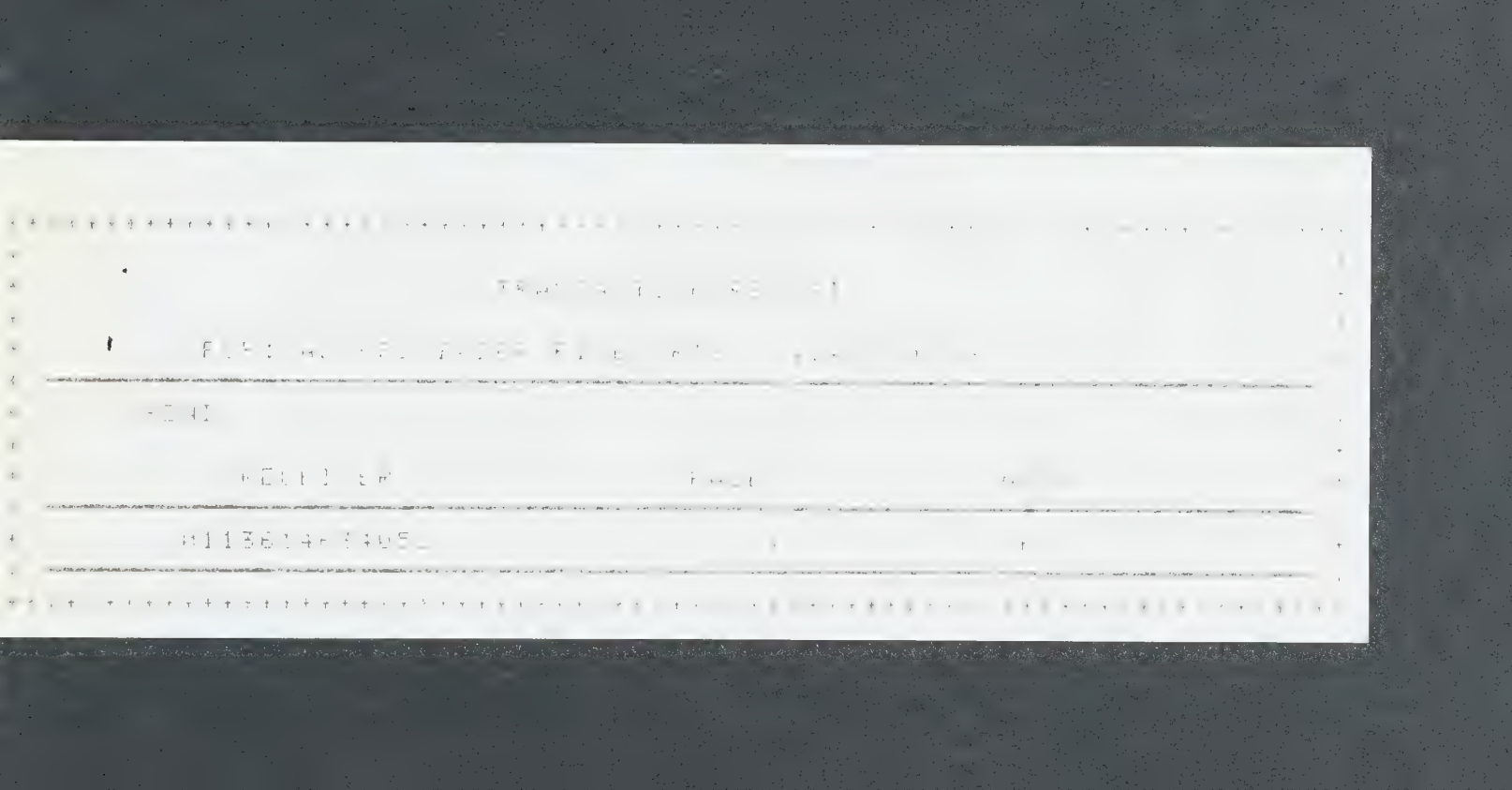
Dear Professor Dr. Hargittai:

In response to your fax of yesterday, I sent you a copy of my autobiography to Budapest by air-mail yesterday.

With all good wishes, I remain,

Yours sincerely,

AB/cw



BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4041, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred Bader
2961 North Shephard Avenue
Milwaukee, WI 53211

August 29 [illegible]
Fax 1-414-277-0709

Dear Dr Bader

Thank you very much for your letter of August 25. Sending my letter of August 14 [illegible] registered mail must have been my mistake

I am very pleased by your interest in The Chemical Intelligencer I am going to send you the first and second issues by mail. I hope you'll be receiving them soon I'll appreciate [illegible] comments you might care making about the magazine

I was happy to be meeting also, however briefly, with David Walton last October during [illegible] visit to the University of Essex

Thank you very much for offering to send me your book to my first location of my visit in the U. S. in November. I shall be arriving just one week prior to our meeting and to a very [illegible] schedule. May I suggest, instead that please, send it to me right away to Budapest? I [illegible] would give me more time to read it. Thank you very much

I shall be very much looking forward to your book and to our meeting on November [illegible]

Yours sincerely,

István Hargittai

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary

FAX FROM:

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

A Chemist Helping Chemists

September 18, 1995

Via Facsimile: 36-1-463-4052

TO: Professor Dr. Istvan Hargittai
Professor of Chemistry
Budapest Technical University

Dear Professor Dr. Hargittai:

Thank you so much for your letters of September 3rd and 6th, for the first two issues of *The Chemical Intelligencer* (to which I am now subscribing) and for your book, *Symmetry*, which I look forward to reading soon.

Also, of course, we very much look forward to seeing you and Mrs. Hargittai in Milwaukee on Thursday, November 9th.

With all good wishes, I remain,

Yours sincerely,

AB/cw

Ofc.Ph.: 414/277-0730
Ofc.Fax: 414/277-0709

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BUDAPEST TECHNICAL UNIVERSITY
Institute of General and Analytical Chemistry
Head of Institute Dr. István Hargittai, Professor of Chemistry
Phone (36-1) 463-4041, Fax (36-1) 463-4052, E-mail hargittai@ch.bme.hu

Dr. Alfred Bader
2961 North Shephard Avenue
Milwaukee, WI 53211

September 3, 1995

Dear Dr. Bader:

Thank you very much for your book. It arrived Friday and I almost finished its first reading. I did this rather fast, it was truly exciting, and I'll have to read it again, more slowly. As I was leaving today (Sunday) for my office, my wife just started reading it. She is a fellow chemist. Then our son, a doctoral student of organic chemistry in the U.S. but currently visiting with us, will have it as a next reader.

I am very much taken by your story. There are lots of crossing points in our lives but even without them the book would be immensely interesting to me. I am Jewish and we spent some time of our deportation in Vienna. I was three and a half.

Having learned a lot now about you did not decrease my interest in the interview a bit, on the contrary!

The book, that is, your life is thought provoking for me a great deal. I can't even attempt to make a list of these thoughts. However, let me mention two. One is that I often wonder about the inefficient and wasteful way scientific publishers operate, and my feeling was that scientist authors could do a much better job of it, if combined with being a good businessperson, just like there must be a tremendous difference between running a chemical company by a real chemist or running it just like any other business. The other thing I wanted to mention is that the story about the benzene formula reminded me of the Italian chemist Paternò who, it appears, preceded van't Hoff and Le Bell, and possibly even Hassel and Barton as regards the tetravalency of carbon and conformational properties. The story is less controversial though but in any case I also have the strong feeling that we should care about these things and for our own sake as much as for those who we think should be getting more credit. I am enclosing a reprint of a recent paper where Paternò and his findings are mentioned.

Also, as a token of appreciation, I have asked the publisher of one of our recent books, Symmetry - A Unifying Concept, to send you a complimentary copy. This is our only book for the general public (so far), and I hope that not only you but possibly Mrs. Bader would also become interested in it.

I hope that the first two issues of The Chemical Intelligencer have reached you in the mean time. The mail worked very well for your book.

Yours sincerely,

Budapest, XI. Szt. Gellért tér 4. H-1521, Hungary