DIRECTIONS IN
THEORETICAL CHEMISTRY

A workshop supported by the National Science Foundation

Snowbird, Utah

April 22-24, 1986

Organizer:

Professor Jack Simons

Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Additional copies of this
report are available from:

Chemistry Division
National Science Foundation
Washington, DC 20550

I. The Workshop Format and Findings

During the week of April 21-25, 1986 a scientific conference was held at Snowbird, Utah. The so-called SNOWBEL conference was focused on "the interface between electronic structure and chemical dynamics". This meeting was held under the auspices of the Sanibel Symposium organization, Professors P. O. Löwdin, Y. Öhrn and J. Simons served as its coorganizers. More than one hundred individuals (representing theoretical and experimental chemistry as well as computer and materials science and funding agencies) took part as registered participants. Scientists from industry, government laboratories, academic institutions and foreign research institutes were present. Ph.D. students, postdoctorals, and independent junior and established research workers were broadly represented in the participant list which is shown below. The scientific program schedule is reproduced on pg. 7.

Ludwik Adamowiz
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

George Adams
Ballistic Research Laboratory
SLCBR-IB-I
Aberdeen Proving Ground
Maryland 21005-5066

Noah Adams
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Hans Agren
Institute of Quantum Chemistry
University of Uppsala
P.O.B. 518, S-75120 Uppsala, SWEDEN

Michael Allan
Institut de Chimie Physique
de l'Universite
CH-1700 Fribourg
SWITZERLAND

Jan Almlof
Department of Chemistry
207 Pleasant Street
University of Minnesota
Minneapolis, MN 55455

Ajit Banerjee
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Rodney J. Bartlett
Quantum Theory Project
369 Williamson Hall
University of Florida
Gainesville, FL 32611

Rudy Baum
Chemical and Engineering News
261 Capricorn Way
Oakland, CA 94611

William Breckenridge
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Joseph Carpenter
Martin Marietta Energy Systems, Inc.
P.O. Box X, Bldg. 4500S, MS-Z60
Oak Ridge, TN 37831

Grzegorz Chalasinski
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

David Chandler
Department of Chemistry
University of California
Berkeley, CA 94720

Sally Chapman
Department of Chemistry
Barnard College
Columbia University
New York, NY 10025

Vernon Cheney
The Upjohn Company
Kalamazoo, MI 49001

Erik Deumens
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Jimmie Doll
University of California
Los Alamos Scientific Laboratory
Los Alamos, NM 87545

Thom Dunning
Chemistry Division
Argonne National Laboratory
Argonne, IL 60439

James Eberhardt
CE-12 Energy Conversion Technology
Department of Energy
Mail Stop: 5E-052
Washington, DC 20585

Paul Engelking
JILA
University of Colorado
Boulder, CO 80309

Julio Facelli
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

William Fink
National Science Foundation
1740 R Street, N.W.
Washington, DC 20006

George Fitzgerald
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Regina Frey
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

David Funk
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Jean Futrell
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Savas Georgiou
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Mark Gordon
Department of Chemistry
North Dakota State University
Fargo, ND 58105

William Hase
435 Chemistry
Wayne State University
Detroit, MI 48202

Janice Hayden
Digital Equipment Corporation
One Iron Way, MR02-3/M91
Marlboro, MA 01752

Eric Heller
Department of Chemistry
University of Washington
Seattle, WA 98195

Dick Hilderbrandt
San Diego Supercomputer Center
GA Technologies Inc.
P.O. Box 85608
San Diego, CA 92138

Jeffrey Hudgens
Chemical Kinetics Division
National Bureau of Standards
Gaithersburg, MD 20899

Sally Hunnicutt
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

James Hynes
Department of Chemistry
Box 215
University of Colorado
Boulder, CO 80309

Kenneth Janda
CB 135
University of Pittsburgh
Pittsburgh, PA 15260

Kenneth Jordan
Department of Chemistry
University of Pittsburgh
Pittsburgh, PA 15260

Joyce Kaufman
Department of Chemistry
Johns Hopkins University
Baltimore, MD 21218

Rick Kendall
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Andrew Komornicki
Polyatomics Research Institute
1101 San Antonio Road, Ste. 420
Mountain View, CA 94043

Kenneth Kulander
Lawrence Livermore National Lab
P.O. Box 808, Mail Code L-487
Livermore, CA 94550

Bill Laidig
Miami Valley Laboratory
P.O. Box 39175
Cincinnati, OH 45247

Stephen Langhoff
NASA/Ames Research Center
Mail Stop 230-3
Moffett Field, CA 94035

Luc Lathouwers
Dienst Teoretische Natuurkunde
RUCA, Groenenborgerlaan 171
202 Antwerp, BELGIUM

Walter Lauderdale
AFRPL/LKLR, Stop 24
Edwards AFB, CA 93523-5000

Stephen Leone
JILA, Campus Box 440
University of Colorado
Boulder, CO 80309

William Lester
Department of Chemistry
University of California
Berkeley, CA 94720

Eugene Levin
Mail Stop 230-5
NASA Ames Research Center
Moffett Field, CA 94035

John C. Light
Department of Chemistry
University of Chicago
5640 S. Ellis Avenue
Chicago, IL 60637

Jan Linderberg
Department of Chemistry
Aarhus University
DK-8000 Aarhus C, DENMARK

W. Carl Lineberger
JILA, Campus Box 440
Boulder, CO 80309

Per-Olov Löwdin
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Mattic Maricq
Department of Chemistry
Brown University
Providence, RI 02912

Jeffrey Marks
P.O. Box 92957
The Aerospace Corporation
Los Angeles, CA 90009

Richard Martin
Los Alamos National Laboratory
MS J569, Theoretical Division
Los Alamos, NM 87544

Edward McCullough
Department of Chemistry
and Biophysics 0300
Utah State University
Logan, UT 84322

Cliff Merrow
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

David Micha
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Josef Michl
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Donald Miller
E328/121A
DuPont Company
Wilmington, DE 19898

Michael Morse
Department of Chemistry
University of Utah
Salt Lake City, UT 84112'

Jules Moskowitz
Department of Chemistry
4 Washington Avenue
New York University
New York, NY 10003

David Nesbitt
JILA
University of Colorado
Boulder, CO 80309

Douglas O'Neal
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Stephen O'Neil
JILA, Campus Box 440
University of Colorado
Boulder, CO 80309

Ceferino Obcemea
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Yngve Öhrn
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Steve Oslon
Floating Point Systems
3601 Murray Blvd.
Beaverton, OR 97005

William Parkinson
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Mark Ratner
Department of Chemistry
Northwestern University
Evanston, IL 60201

Thomas Rescigno
Lawrence Livermore National Lab
P.O. Box 808
Livermore, CA 94550

Stephen Rodgers
Edwards Air Force Base
AFRPL, stop 24/LKLR
Edwards AFB, CA 93523

Ernst Ruch
Institut fur Quantenchemie
der Freien Universitat Berlin
Holbeinstr. 48
D-1000 Berlin 45, WEST GERMANY

Andrew Sadlej
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Erland Sangfelt
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

George Schatz
Department of Chemistry
Northwestern University
Evanston, IL 60201

Arthur Sedlacek
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Ron Shepard
Chemistry Division
Argonne National Laboratory
Argonne, IL 60439

Randall Shirts
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Per Siegbahn
Institute of Theoretical Physics
University of Stockholm
Vanadisvagen 9
S-11346 Stockholm, SWEDEN

Jack Simons
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Ellen B. Stechel
P.O. Box 5800
Sandia National Laboratories
Albuquerque, NM 87185

Clifford Stodden
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Krzysztof Szalewicz
Quantum Theory Project
362 Williamson Hall
University of Florida
Gainesville, FL 32611

Howard Taylor
Department of Chemistry
University of Southern California
University Park
Los Angeles, CA 90089-0482

Hugh Taylor
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Donald Truhlar
Department of Chemistry
University of Minnesota
207 Pleasant Street
Minneapolis, MN 55455

John Tully
AT&T Bell Laboratories
Room 1A-357
Murray Hill, NJ 07974

Piet Van Leuven
Dienst Teor. Wisk. Natuurkunde
RUCA, Groenenborgerlaan 171
2020 Antwerp, BELGIUM

Gabriel Vazquez
Instituto de Fisica, UNAM
Cuernavaca Laboratory, AP 139-B
62190 Cuernavaca, Mor., MEXICO

Jiang Wang
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Donna Wetzel
Department of Chemistry
Stanford University
Stanford, CA 94305

Donald Whitehead
Scientific Computer Systems
25195 S.W. Parkway Avenue
Wilsonville, OR 97070

Carles Wight
Department of Chemistry
University of Utah
Salt Lake City, UT 84112

Erich Wimmer
CRAY Research, Inc.
1333 Northland Drive
Mendota Heights, MN 55120

Curt Wittig
Department of Chemistry
University of Southern California
University Park
Los Angeles, CA 90089

Francis Wodarczyk
AFOSR/NC
Bolling AFB, DC 20332-6448

Robert Wyatt
Department of Chemistry
University of Texas
Austin, TX 78712

David Yarkony
Department of Chemistry
Remsen Hall
Johns Hopkins University
Baltimore, MD 21218

Danny Yeager
Department of Chemistry
Texas A & M University
College Station, TX 77843

Final Snowbird Conference Schedule

Sessions are held in the Cottonwood Conference Center. There are three sessions per day: A: 8:15-10:30 a.m., B: 3:30-6:30 p.m., C: 8:30-11:00 p.m. The time between sessions is free for informal get togethers, meals, skiing, etc.

Monday 8:00-8:15 Opening Remarks

Session A

Thom Dunning, "Reaction Paths for Chemical Reactions"
Per Siegbahn, "The calculation of potential energy surfaces for homogenous and heterogenous catalytic processes"
Bill Lester, "Quantum Monte Carlo for Molecules: Energies and Other Properties"

Session B

Jan Almlof, "The Calculation of Accurate Infrared Vibrational Intensities"
Rod Bartlett, "Analytical Derivative Methods and Coupled Cluster Theory"
Ed McCullough, "MCSCF and MCSCF-CI Calculations on Transition Metal Diatomics Using Numerical Basis Sets"
Rich Martin, "Model Studies of the Epoxidation of Ethylene on Silver"

Session C Poster Session #1

Tuesday

Session A

Ken Jordan, "Temporary Anion Resonances in Polyatomic Molecules"
David Yarkony, "Recent Advances in the Theoretical Treatment of Nonadiabatic Processes"
Michael Allan, "Some recent experiments on inelastic electron-molecule collisions at low energies"

Session B

David Chandler, "Field Theoretic Approaches to Solvation"
Mark Ratner, "Semiclassical Self-Consistent Field Calculations of Vibrational Dynamics"
Casey Hynes, "Dynamical Aspects of Reactions in Solution"
Jules Moscowitz, "Monte-Carlo Green's Function Methods in Electronic Structure"
Eric Heller, "Chaos, Quantum Mechanics, and the Mexico City Earthquake"

Session C NSF Workshop Session #1

Wednesday

Session A

Steve Leone, "Dynamics of Ion-molecule Reactions"
Jean Futrell, "Reaction Dynamics of Low Energy Charge Transfer Reactions"
Carl Lineberger, "Photodetachment Probes of Electronic Structure and Vibration, Rotation-Electronic Coupling in Anions"

Session B

Bill Breckenridge, "Half-Collision Versus Full-Collision Dynamics: Van der Waal's Complexes of Electronically Excited Atoms"
Don Truhlar, "Electronic Structure and Dynamics Calculations: Inelastic and Reactive Collisions"
George Schatz, "The Dynamics of Reactions which Produce Highly Excited Intermediates or Products: The Need for Better Global Potential Surfaces"
Bob Wyatt, "Dynamics of the Li + HF Reaction"

Session C NSF Workshop Session #2

Thursday

Session A

Curt Wittig, "Reactions in Clusters"
Jim Doll, "Theoretical Studies of Hydrogen Diffusion"
John Tully, "Dynamics of Gas-Surface Interactions"

Session B

Ken Janda, "Measurements and Calculations on the Vibrational Predissociation of $NeCl_2$"
George Lie and Enrico Clementi, "Global Computations: Quantum Chemistry, Statistical Mechanics and Continuum Mechanics"
Randy Shirts, "Intramolecular Vibrational Rotational Dynamics on Model Potential Surfaces"
Andy Komornicki, "*Ab Initio* Vibrational Spectroscopy: Computational Aspects and Applications"

Session C NSF Workshop Session #3

Friday

Session A

Yngve Öhrn, "Dynamics of Nuclei and Electrons Using the AGP Coherent State"
Jan Linderberg, "Reactive Scattering in Hyperspherical Coordinates"
Bill Hase, "Potential Energy Surface Properties and Intramolecular Vibrational Energy Relaxation in Benzene"

Session B

Per-Olov Löwdin, "Towards a Theory of Chemical Reactions"
Sally Chapman, "Proton transfer reactions: Heavy-Light-Heavy dynamics in ionic systems"
Howard Taylor, "Energy Localization in Molecules: Dynamic Causation and Spectroscopic Consequences"
David Micha, "Extensions of the time-dependent Hartree-Fock Method and applications to atomic collisions"

As an integral part of the Snowbel conference, a three-session National Science Foundation funded workshop was held on Tuesday, Wednesday and Thursday evenings. It's primary purposes were to examine and make constructive recommendations concerning the status and state of health of theory within chemistry and of chemistry within science and society. To focus the discussion of the workshop, at least initially, a set of eight questions were posed for consideration. These eight questions are listed below.

1. **What is the present state of health of theory within chemistry?**

2. **Where has theory contributed substantially and significantly to research in chemistry and in related disciplines?**

3. **Where should theoretical chemistry be focusing its efforts so as to have greater impact in science and technology?**

4. **What steps can be taken to so focus theory's efforts and what resources are needed to achieve this?**

5. **What is the present image of chemistry in society?**

6. **What should and can be done to improve this image?**

7. **In what directions should chemistry research be evolving so as to maximize both innovation and its impact on related disciplines?**

8. **What improvements are needed in our educational process to better prepare our students for productive careers in theory?**

The NSF workshop began on Tuesday evening with a forty minute introductory and overview session in which the workshop organizer Jack Simons outlined to the more than one hundred participants the format, scope, and goals of the workshop. Subsequently, the participants were divided into eleven working groups of approximately ten persons per group. For the remainder of the Tuesday session, these working groups met individually to discuss the above eight questions. During the first working group meetings all participants responded to a questionnaire consisting of twenty-five written statements which were designed to provide further directions to their initial discussions. The twenty-five statements along with numerical data summarizing the responses of all participants are displayed below.

Questionnaire Response Summary

Statement	Ave[a]	Std[b]
1. Chemistry is a "central science" which generates new spin-offs and impacts many other disciplines.	7.17	0.62
2. Theory is maturing and, as a result, contributing more to chemistry than it did ten to twenty years ago.	6.75	1.35
3. Theoretical chemistry plays much the same role in chemistry as theoretical physics does within physics.	-3.50	1.26

4.	Chemists should carry out more of their work in centralized interdisciplinary research centers.	-2.08	2.32
5.	Theoretical chemists should develop closer ties with scientists in the chemical, biotechnological, and materials industry.	5.58	1.10
6.	The NSF funded supercomputer initiative is a good idea which greatly benefits theoretical chemistry.	4.17	1.57
7.	Theoretical chemists need to develop centers for work in theory much like the Santa Barbara theoretical physics institute.	3.67	1.57
8.	Computer programs developed for research by theoretical chemists should be more openly circulated to the general chemistry research community.	3.83	2.53
9.	Theoretical models and concepts should be emphasized to a larger extent than at present in the undergraduate chemistry curriculum.	5.57	1.86
10.	The public thinks of Bhophal, acid rain, and chemical and nuclear waste when they think of "chemistry".	5.33	1.37
11.	The NSF's new initiatives (e.g., supercomputers, computational mathematics, life processes, etc.) provide net benefit to the basic research effort which NSF is supposed to fund.	4.33	1.37
12.	The following constitute major intellectual frontiers: understanding chemical reactivity, chemical catalysis, chemistry of life processes, chemistry around us, chemical behavior under extreme conditions.	5.67	1.11
13.	Priority should be given to the following research frontiers: understanding chemical reactivity, chemical catalysis, chemistry of life processes, chemistry around us, chemical behavior under extreme conditions.	3.17	2.11
14.	New mechanisms and new incentives should be sought for strengthening links between industrial and academic research.	5.67	0.94
15.	Industry should increase its support for university fundamental research in the chemical sciences.	6.17	0.90
16.	The federal investment in chemistry should be raised to be commensurate with the practical importance of chemistry, both economic and societal, and with the outstanding opportunities it now offers.	7.00	1.83
17.	Within molecular dynamics, areas of major importance are: fast chemical processes in real time, energy	6.33	1.25

transfer and movement, state-to-state chemistry, multiphoton and multiple photon excitation, mode-selective chemistry, ab initio calculations of reaction surfaces, and theory of reactions.

18.	Lasers have peaked in their applications to chemistry.	-5.33	2.62
19.	Chemistry involves too much instrumentation these days, we need to focus on what can be done with less complicated and expensive means.	-5.58	1.64
20.	The following areas represent new horizons in chemistry: biotechnology, high-technology ceramics, advanced composites and engineering plastics, photo-imaging, microelectronic devices, molecular-scale computers.	3.67	1.11
21.	We need to convince more highly talented students to pursue careers in areas where chemistry is evolving.	6.92	1.88
22.	We need to convince more excellent students to pursue degrees in joint experiment-theory projects.	4.17	2.03
23.	The chemical, drug, electronics, and computer industry needs to hire more theoretical chemists.	5.33	1.80
24.	Chemists have done wonders in losing their identity in the rest of science (see handout).	0.92	3.06
25.	We need to provide our students with more mathematics, physics, and computer use education.	7.58	0.89

a) Average over approximately 100 responses with 10 representing strong agreement, 5 mild agreement, 0 neutral, -5 mild disagreement, and -10 strong disagreement.

b) Standard deviation within the approximately 100 responses. Relatively small standard deviations are taken to mean that a consensus position exists.

In the first half of the Wednesday evening NSF workshop session, spokespersons from each of the eleven working groups gave brief (3-10 minutes) reports of the preceding evening's group analyses. In particular, each of these spokespersons (Steve Leone, George Schatz, David Micha, John Tully, Jim Doll, John Light, Thom Dunning, Bill Lester, Ken Janda, Ken Jordan, Andy Komornicki) presented their group's consensus (or lack thereof) positions on the eight questions raised above. They also brought up several new issues which formed the basis for discussion from the floor. Having heard from each working group, the participants were once again asked to meet as individual working groups to further refine their positions on the eight focal questions as well as on other issues which arose earlier in the Wednesday session. The remainder of the Wednesday session was devoted to these working group analyses.

The third and final NSF workshop session was held on Thursday evening. At this get together Jack Simons summarized the consensus positions which he felt were reached during the preceding evening's discussions. Several participants then made statements expressing their own views concerning various of the consensus positions. The eleven working group spokespersons presented to Jack Simons written summary responses to the original eight questions as well as remarks pertaining to several other issues which arose during the Tuesday and Wednesday sessions. From these written summaries the statements and points of view judged to represent consensus or at least wisely held positions were extracted and are tabulated below.

Responses to the Eight Questions Representing Widely Held Positions[a]

1. What is the present state of health of theory within chemistry?

Academic chemists as a whole may not appreciate the role of theorists. But, its health is quite impressive recently because of two trends. (1) People are more problem-oriented, as opposed to technique-oriented, (2) People are attempting more complicated problems, even though the results may not come out perfectly. Its health is better today because there is a great deal of communication between experimentalists and theorists too.

The health is generally positive but there are areas of concern.

On the positive side are:

a) Good progress in using theory in new applications.
b) Several groups of theoreticians have evolved (and done well) at government labs and industry.

On the negative side are:

a) The percent of academic jobs going to theorists is static.
b) A decline in student quality.

The health of theoretical chemistry is better than ever. It is more appreciated; these are intellectually very exciting times for it. It could be doing even better with more stable support.

Modern chemical theory is rapidly developing, if young, contribution to advancement of chemical science (strong, vibrant).
Due to combination of advances in theoretical and conceptual understanding of fundamental factors which govern chemistry and increasing access to needed computing resources.

We all agreed that in recent years the image of theoretical chemists has improved considerably. In part this is due to the increasing interactions between theorists and experimentalists. Also important is the fact that with increasing frequency, theoretical predictions are now preceding experiment. In the past theoretical calculations tended to follow experimental measurements. We believe that it is significant that there is considerable crossing of theoretical boundaries. Stat. mechanicians are getting interested in the electronic structure problem, electronic structure theorists are getting involved in studies of solvation and dynamics, and, finally, the dynamicists are interacting very strongly with the electronic structure theorists.

2. Where has theory contributed substantially and significantly to research in chemistry and in related disciplines?

Theory has contributed significantly in a number of areas of which are listed below:

The most noticeable is the use of electronic structure calculations in the predictions and investigations of molecular structures.

Conformational analysis, as applied to polymers, and biological systems. Present efforts at drug design are largely based on this concept:
surface physics, and surface chemistry
theory of rate processes
liquid theory
atmospheric chemistry

Theory has contributed to pharmacology, polymers, high-energy compounds; new methods for solving the Schrodinger equation.
"Theory is the difference between alchemy and chemistry"

Theory provides the framework in which experiments are conceived and interpreted.

As experiments become more sophisticated, interpretation becomes more sophisticated.

Data without a model is not science.

Many examples can be given

MO & VB Theories
Woodward-Hoffmann Rules
Onsager Relation
Phase Transitions
Periodic Chart, Thermodynamics (Boltzmann), Statistical Mechanics

But is such anecdotal evidence appropriate here?

Quantitative Predictions

Now widely recognized that theory has something concrete, if still not as quantitative as would like, to say to experimentalists.

Theory provides the language that is used to discuss chemistry and is being increasingly accepted as providing quantitative tools to study problems that are often inaccessible to experiment. In general the field is well received in academia although there seems to be a bias against hiring electronic structure theorists. This is hard to understand given the high visibility of electronic structure as evidenced by the high citations of Pauling and Pople; the popularity of Bill Goddard and Fritz Schaefer and the widespread use of quantum chemistry routines. Theory is being widely adapted by chemical and drug companies via computer modelling routines. There is not enough recognition of the value of chemical theory by the portions of national labs and high tech industries dominated by applied physicists.

We then turned to the issue of the image difficulties and status of theoretical chemistry within the overall discipline of chemistry. Several individuals in our group expressed the opinion that the situation of theory in chemistry has been different from that in physics in that theoretical chemists have felt more "pressure" to continually justify themselves to their experimental colleagues. Also many chemistry departments have only 1-2 theorists, while it is rare to find a physics department with so few theorists. Given the increasing synergism between theorists working in different areas and the recent advances made in theory a good case might be made for an increase in the number of theorists.

Current contributions are apparent, particularly at national laboratories (laser isotope separation, chemical lasers, ...) and now industry (drug synthesis routes, "quantum pharmacology", etc.), etc.

A considerable amount of discussion focused on the distinction, if any, between the utilization of theoretical techniques to answer specific problems and the support of basic research to <u>develop</u> techniques. We emphasize that even in the age of supercomputers, the development of abstract theory, theoretical models, and improved approaches and techniques is clearly essential. Theoretical chemistry should be broadly construed with respect to application areas, including biochemistry, polymer physics, etc.

3. Where should theoretical chemistry be focusing its efforts so as to have greater impact in science and technology?

Future focus: do not focus!!!
Rather than focus, we should bring under the umbrella of chemistry the diverse fields which have been spun off from chemistry over the past few years. This would bring them under the unifying principles which chemistry offers.
- - chemistry by its very nature is a unifying science.
We should not focus on any specific areas, but develop fundamental theory and concepts.

We assume that a balance between focused and unfocused polymers work will be economically driven. Some interesting focused areas would be:
Tribology - the study of wear and friction.
"Materials by design"
Theory has to make first tries at larger, more complex systems, which seems to be what most chemistry cares about.

<u>Note</u> Chemistry outside of academia is not so divided along division lines. In companies, theorists work along side engineers, physicists, to approach problems of interest.

We strongly recommend that the theory section of the ACS collect, edit and augment the various computer graphics and movies that have been developed. The videos should be adapted for use by students at each level and for presentation to the public. Computer calculations should be adapted for use in undergraduate education.

Both popular magazines and PBS should be used to bring the exciting new problems of chemistry to the public.

Universities need to establish better ties with the chemical industry. Faculty should be more active in local ACS sections in order to meet industrial scientists. Seminar programs should be established to introduce students at all levels to the activities of industrial scientists.

Our group is generally against attempts to focus research in theory. We feel that diversity and creativity must be fostered by the NSF. We don't support NSF creation of national theory centers which would lower individuality in research.

We currently have a "mixed economy" in determining focal areas and directions. Most (not all) on the committee felt that strong efforts to focus theoretical chemistry on specific areas, while perhaps productive in the short run, probably would not be healthy in the long run.

One consensus suggestion was to encourage topical (perhaps interdisciplinary) workshops on unresolved problems (vague to specific; theo. to expt.). Cross disciplinary initiatives, etc. Some doubt was expressed that theoretical chemists understand the value (or lack thereof) of what they do, do not face real problems of the real world, etc. All on the committee felt the stimulation of more collaborative focus on unresolved problems would be valuable. Presumably these would be short and finite team workshops, collaborations, etc. which are not strongly institutionalized.

No other real discussion of mechanisms occurred.

4. What steps can be taken so as to focus theory's efforts and what resources are needed to achieve this?

Increased collaboration between subdiscipline of theory and increased collaboration between theory and experiment should be encouraged.

Need access to necessary computer resources:

Front-end processors (VAX, workstations, etc.) with greatly enhanced graphics capability and auxilliary equipment.

Back-end processors (FPS, CRAY, CYBER, etc.) with large memories and fast CPU's.
Equivalent of CRAY X-MP
Need ~ 10 hrs./week for researchers involved in computationally-intensive projects (more for groups)

Effective use of computers is manpower intensive.

Workshops are very effective at focusing on problems and bringing everyone up-to-speed.

5. What is the present image of chemistry in society?
6. What should and can be done to improve this image?

Together - Most people have simple-minded ideas about chemistry. Our belief is most people are neutral to chemistry. A TV series though on chemistry would do much to enhance the image of chemistry. Upgrade displays in museums if necessary.

There is a difference between the image of chemists (academic types) and chemicals, with the latter being very bad.

This does not mean that academic types should refrain from helping to improve the image of chemistry in general.

We need

a) A TV show (NOVA) about chemical reactivity

b) modernized chemistry educational aids:

PC's capable of ab initio calculations exploratorium programs.

c) lecture/demonstrations in theory for high school teachers.

Image of chemistry is not good. Find several "Carl Sagan"s to promote theoretical chemistry.

Chemists should take a more active role in bringing accomplishments and excitement of chemical research to educated public.

NOVA programs

Articles in Scientific American and Science 86

C&E News - Too many of research note have to do with physics and biology.

How can this be done?

Better choice of terminology.

Chemists not represented well in television shows, etc. (even Sesame Street).

Theory (and chemistry in general) needs to be more effectively brought before the public. This should start at the Junior High level in order to help attract bright young people to chemistry. The exciting advances in theory need to be incorporated into high school course work and the freshman year to improve the image of the field.

We strongly recommend that the theory section of the ACS collect, edit and augment the various computer graphics and movies that have been developed. The videos should be adapted for use by students at each level and for presentation to the public. Computer calculation should be adapted for use in undergraduate education.

Both popular magazines and PBS should be used to bring the exciting new problems of chemistry to the public.

Universities need to establish better ties with the chemical industry. Faculty should be more active in local ACS sections in order to meet industrial scientists. Seminar programs should be established to introduce students at all levels to the activities of industrial scientists.

Our group is generally against attempts to focus research in theory. We feel that diversity and creativity must be fostered by the NSF. We don't support NSF creation of national theory centers which would lower individuality in research.

We first discussed the image of chemistry in the society at large. We were concerned not only with the bad publicity that chemistry has received due to environmental problems but also with the lack of "good publicity". In recent years various chemical companies have dropped the word "chemical" from their name or from their advertising slogans. A good example of this is Dupont which has dropped the "chemistry" from their slogan "Better living through chemistry". Also some drug companies have begun to refer to the misuse of drugs as "chemical abuse". It appears that the word chemistry has acquired such a bad image that the chemical industry is rapidly trying to distance itself from references to "chemistry". In doing so they are making the problem worse. (Is the situation so bad that we in universities should relabel ourselves as "Molecular Scientists"?)

Compared to biology, physics, astronomy, and electronics research development in chemistry receives very little exposure in newspapers, general science magazines such as Science 86, and on science-related TV programs such as NOVA. We feel that it is crucial for the chemistry community to get more exposure through these channels. Other opportunities include exhibits at museums, particularly those with hands-on exhibits as well as increased involvement (perhaps by giving demonstrations or providing movies of computer simulation of chemical processes) with High School and Junior High School chemistry and science courses.

We also felt that chemistry makes a very important contribution to a wide range of other disciplines including materials science, biology, and electronic device fabrication. Consequently, we should take every opportunity to educate the public as to the nature of chemistry's role in these other areas.

7. In what directions should chemistry research be evolving so as to maximize both innovation and its impact on related disciplines?

The Pimentel report should be supported here.

Answered by the Pimentel report, except that chemical dynamics was not sufficiently emphasized in Pimentel Report.

Theoretical chemistry is likely to evolve into two (strongly connected) branches. The first, the development of new concepts and new computational techniques, will continue as present. The second, modelling, is in its infancy today. But with increased hardware and software capabilities, computer modelling is likely to become a very significant activity in chemical research. It is likely that the predictive power of modelling will be sufficient that modelling will replace experiment as the method of choice for obtaining accurate data for continually expanding classes of chemical problems. We have not reached this situation today except for the simplest chemical systems. But the importance of modelling is likely to grow very significantly over the next decade or two. This will probably lead to an increase in the fraction of "theorists" - in chemistry departments and industrial labs. It will also probably be met with resistance from experimentalists and "pure" theorists as well. It will be advantageous for chemical theorists to be aware of this evolution and prepare for it. Systematic develpment with continual testing against experiment must be demanded. "Black box" use must be avoided. And most importantly, false claims and adversary relationships with experimenters must be avoided.

The major limitation of theoretical chemistry is the ability to address large systems using current electronic structure techniques. Even with tremendous improvements of computer hardware, extensions of current CI techniques will peter out at systems only a factor of 10 or 100 larger than current limitations. This is too small to handle most biological, large molecule, condensed phase or surface questions of current interest. A major breakthrough is needed. Monte-Carlo techniques are a breath of fresh air in this regard. They may, in the end, not prove competitive with CI methods, but there is hope - it is a totally new direction that shows promise. Kenneth Wilson's renormalization group machinery, although initially appearing to be awkward for electronic structure problems, may also have promise. New ideas, however strange at first, should be encouraged at the expense of incremental developments in traditional CI methods. This, of course, is a specific example of the general desire to give more support to risky new ventures. Hiring, funding, promotion and tenure decisions must give greater weight to innovation, potential import and risk, and be less dependent on the length of publication lists.

We currently have a "mixed economy" in determining focal areas and directions. Most (not all) on the committee felt that strong efforts to focus theoretical chemistry on specific areas, while perhaps productive in the short run, probably would not be healthy in the long run.

One consensus suggestion was to encourage topical (perhaps interdisciplinary) workshops on unresolved problems (vague to specific; theoretical to experimental) - Cross disciplinary initiatives, etc. Some doubt was expressed that theoretical chemists understand the value (or lack thereof) of what they do, do not face real problems of the real world, etc. All on the committee felt the stimulation of more collaborative focus on unresolved problems would be valuable. Presumably these would be short and finite team workshops, collaborations, etc. which are <u>not</u> strongly institutionalized.

No other real discussion of mechanisms occurred.

8. What improvements are needed in our educational process to better prepare our students for productive careers in theory?

There should be an increased emphasis on physics and mathematics in the chemistry curriculum.
It is largely felt that the present structure of curricula does not respond quickly enough, if at all to new areas which are spawned by research.

In p. chem. lab (undergraduate) do some theory calculations.
Introduce terminology early.
The stat. mech. which we usually teach is not modern. Texts will have to change.
Combined math-chem. courses may be needed.
Need broader exposure of how theory is applicable for students.
We support manpower and other financial and computing resource needs.

Generally this is true for all disciplines of chemistry, however, not just theory.

Based on experience with the ACS Committee on Professional Training, it is tough to change anything. However it would be nice to have all chemistry undergrads. learn about computing, and with the aid of PC's running ab initio programs, they might even learn about theory as well.

Teach methodology: how to do theory.
Encourage deep knowledge of computing.
Provide for continuing education; paid by employers?
Contact the ACS Committee on Professional Training to require two semesters on numerical methods and computing for ACS-approved degrees in chemistry.

Need to exploit computers to give students a better understanding of structure and dynamics - not programs that are just rehashing of textbooks, but innovative programs which make heavy use of graphs, etc. to provide detailed look at chemical reactions, solvation, etc.
Need better background in applied mathematics.
Real problem, at least in the near future, will be lack of jobs for theoreticians.
Need better grounding in fundamentals, mathematics, physics as well as chemistry.

Clearly excellent students are necessary if theory is to remain healthy. Math and Physics skills need to be emphasized at the pre-college level so students are capable of handling college and grad. school in theory. Students must be attracted to chemical theory via the public activities outlined earlier in this report.

It has been noted that theoretical chemists frequently find it more difficult to obtain research positions, either faculty or industrial, than their experimental counterparts. Some of this is inevitable, at least in industry where competent but non-innovative experimenters can make valuable contributions in relatively routine tasks. There appear to be fewer such routine tasks for theorists. However, another reason which may contribute to the difficulty in obtaining jobs is the overspecialization of some theorists. This results in part from exploitation by their advisors. Students must be given the chance (i.e., required) to obtain a global view of chemistry, interact with experimentalists, pursue problems of chemical import, give seminars, etc. There is almost no chance a person will be offered a job if his or her interview seminar is about a new method for doing three-center integrals. A thesis consisting predominantly of developing code should not be allowed. The pressure of producing felt by advisors does not justify exploitation of students.

Remarks on Other Issues which Attracted Substantial Attention[a]

It is felt that both qualitative and quantitative results have improved a great deal over the past ten years, which gives us a vastly improved understanding of fundamental phenomena. However, the funding is not commensurate with the progress.

For the future, the following are important:

Development of new generation of computers, both desktop workstations and large supercomputers, will have profound, positive impact on theoretical chemistry.
Need to translate sophisticated mathematical models into qualitative models of use to "bench" chemists.
Need additional manpower.
  Will be unable to fully exploit advances in computers without additional manpower.

We concluded that the different areas of theory appear to differ in their effectiveness at communicating their goals to other chemists. Significantly, it was felt that there is a need for electronic structure theorists to better communicate the problems they face (e.g., the steep N dependence) the strategies they are working on to extend the range of systems that can be treated. In interacting with non-experts perhaps more emphasis should be placed on physical concepts instead of on mechanical details.

Finally we discussed the situation with respect to hiring of electronic structure theorists at major universities. Although nearly all the speakers (both experimentalists and dynamicists) at the meeting stressed the need for better potential energy surfaces there seems to be a reluctance on the part of universities to hire electronic structure theorists. Over the last eight years we could not think of any assistant professors in electronic structure theory having been hired at the top 25 universities. Many of the top schools -- MIT, Stanford, Columbia, Colorado, do not have individuals in electronic structure theory. We found this puzzling in light of the significant advances (gradients, pseudopotentials, unitary group approaches to the correlation problem, etc.) and the greatly enhanced computer resources now available.

Some additional computer-related issues come up in our discussions. First, the effective utilization of supercomputers, array processor, parallel processing, and sophisticated graphics will require considerable manpower (i.e. graduate students and postdoctoral fellows). Although the NSF advanced scientific program has spent considerable funds for hardware, and operating costs of the supercomputers, essentially no funds have been made available to the researchers.

The fields of atomic and molecular physics and chemical engineering are apparently facing decreased student enrollments and increasing struggle for research funds. Chemistry is healthier, largely because of its breadth. Its contributions to biology and to materials science, in particular, are so significant that advances in these areas rival in importance those in the core areas of chemistry. Rather than diluting chemistry, excursions into interdisciplinary areas are a major source of strength.

a. These statements are direct or nearly direct (with minor attempts to improve sentence structure only) quotes taken from the eleven working groups' reports.

II. Brief Summary of Findings and Recommendations

The raw data, as represented in the individual participants' responses to the twenty-five questionnaire statements and in the working groups' responses to the eight focal questions, must be read in full to achieve an optimal understanding of the Workshop's main conclusions and recommendations. However, it is useful to extract from these statements a few of the most broadly supported positions.

Using the standard deviations of the questionnaire responses to each of the twenty-five individual statements as indicators of consensus, it can be concluded that the Workshop supports the following conclusions:

1. Chemistry is a "central science" which generates new spin-offs and impacts many other disciplines.

2. Theoretical chemists should develop closer ties with scientists in the chemical, biotechnological, and materials industry.

3. New mechanisms and new incentives should be sought for strengthening links between industrial and academic research.

4. Industry should increase its support for university fundamental research in the chemical sciences.

5. We need to provide our students with more mathematics, physics, and computer use education.

6. The following constitute major intellectual frontiers: understanding chemical reactivity, chemical catalysis, chemistry of life processes, chemistry around us, chemical behavior under extreme conditions.

The opinions expressed by the eleven working groups concerning the eight focal questions are quite diverse. Nevertheless, it seems that the following consensus positions developed:

Relative to Theoretical Chemistry

1. Theoretical chemistry is healthy and its image within chemistry has improved due largely to more extensive interactions with experimental groups and trends toward more problem orientation.

2. Theoretical chemistry has contributed to chemical, drug, and materials research in a myriad of ways. Most importantly, theory is the language in terms of which we view chemical results.

3. No efforts should be made, by funding agencies in particular, to focus theoretical chemical research although collaborative research with industry, which ought to be strongly encouraged and enhanced, is, by its very nature, likely to be more focused.

4. The use of theory for modelling chemical and physical properties and behavior is likely to grow rapidly in the next several years.

5. The number of jobs for theoreticians in university environments seems to be static, although the very best universities tend to have proportionally more theoretical chemists. This is surprising and dismaying in light of the many contributions which theory has recently made. Enhancing the fraction of theoreticians on our faculties would be healthy and beneficial especially in areas where theory is experiencing strong synergistic interaction with experimental research.

6. The Theoretical Chemistry Subdivision of the Physical Chemistry Division of ACS needs to be more aggressive in representing its constituency within chemistry. It should also gather together video movies, educational computer programs, and other tools which would be disseminated to local ACS sections or to colleges, industries, and universities to illustrate what theoretical chemistry is and why it is exciting and useful.

Relative to Chemistry as a Whole

1. The public image of the chemical industry, and perhaps of chemical science, is very bad. Strong steps should be taken to improve this image especially as it pertains to chemical science. Recommended steps include: a TV series on chemistry, updating museum and exploratorium displays, and lectures/demonstrations for high school teachers aimed at showing chemistry's full value to society. Identifying a few "Carl Sagan" like spokespersons would be very valuable.

2. Universities need to develop much closer ties with industry. The local ACS chapters could provide a communication link to begin this process.