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Summary

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The essays that follow are from 20 different individuals, all of them distinguished for their research, and also for their willingness to think broadly about science and its future. Many of them are not known as physical organic chemists, but all of them have used the tools of this discipline in their work, and comment upon the utility of this discipline for the practice of other areas of chemistry as well.

The authors were given great latitude in composing their contributions, and the diversity of approaches that resulted is just what was sought, as it shows the wide range of the field. It is indicative of the evolution of the field that the venerable names of the affiliations of two of the contributors changed during the year this collection was assembled, as the Department of Chemistry at Harvard University became the Department of Chemistry and Chemical Biology, and CIBA-Geigy and Sandoz became the Novartis Corporation. Thus both in academia and in industry institutions change to better reflect the nature of the field, and to anticipate the future.

The theme runs through all of the essays that the future of the field lies in an interdisciplinary approach and that physical organic chemists will use all of the tools available, and will not be fettered to narrow views. Physical organic chemistry will be active in the 21st Century in the elucidation of the interrelation of chemistry and biology, in the design and construction of new materials and molecular devices, in the study of chemical processes in solution, gas, and solid phase, and at extremes of conditions. Computational chemistry will play an increasing role, and new instrumental techniques will be widely utilized. The field of materials will receive increasing attention, particularly in the application of the understanding of the origins of chemical properties and detailed mechanisms of reactions to the design of materials and devices for specific purposes.

Physical organic chemistry will also be increasingly involved in education, in profit-making activities, and in political activity. Courses in physical organic chemistry are taught all over the world to advanced undergraduates and graduate students, and are seen by many outside the discipline as an essential part of the training for individuals who throughout their careers will have to respond in creative ways to an ever-changing science. Teachers will be called upon to provide fundamental understanding and a flexible approach to problem solving so that future challenges can be met. New textbooks that present in a managable fashion the increasingly diversified subject matter of the field will also be needed.

Some are skeptical about the future of physical organic chemistry, and about the use of an exercise such as this. The pessimists who believe the field has no place to progress harken back to some who felt the area was exhausted over 30 years ago, and those individuals were shown to be wrong by unparalleled decades of new achievement.

Those who say we cannot predict the future are correct in one sense, in that we cannot say exactly what will be discovered over given periods of time, or how these discoveries will affect the future direction of research, as well as our everyday lives. We can however be confident that these discoveries will be made, and with less certainty we can often predict which individuals are likely to be most successful. These are those who have made outstanding achievements in the past, and who can articulate what they hope to do in the future. New discoveries will also arise from unanticipated quarters, and given the opportunity new faces will continually join the leaders in the field. While their discoveries will not necessarily be what they expect, scientists have a much better record for clairvoyance than do the economists or politicians, who expect others to produce on demand, while never having to defend their own dismal records of prediction.

Some of the authors (Arnett) touch upon the subject of chemophobia, the irrational fear and distrust felt by some of "chemicals". This has led some chemical companies to drop the word chemistry from their title or slogans. However equally prominent in the popular press are the uniformly positive connotations of having "good chemistry", as applied to movie stars, athletes, musicians, and a host of others. My favorite example is a headline that a football coach was fired for "lack of chemistry", as if this was a gaping void on his academic transcript. The message is that there is widespread appreciation of the value of chemistry, and the public realizes that there are risks and hazards associated with any worthwhile activity, whether it be physical exercise or airline travel.

One theme found in many of the essays (Olah, Fox, Bellus) concerns the value of physical organic chemistry in teaching scientists to be problem solvers, and specific areas for emphasis in graduate research that would be of value to industry and society are noted by Bellus. Arnett notes the role played by chemistry conferences in education and in the spread of knowledge and ideas. Chemistry journals, which have changed very little in the past century, can also be expected to finally make a decisive move away from printed paper as the major means of distribution.

Many of the authors, including Nefedov, Arnett, and Breslow, note that computers, instrumentation, and electronics will have an increasingly large role in the future. Biological chemistry is also sure to increase in importance , as emphasized by Westheimer, Ingold, Breslow, Roberts, and Mukaiyama. Gas phase chemistry, as discussed by Cacace and Schwarz, will also continue as a major field of study, and will be particularly dependent on improvements in instrumentation. This area will be of value for such diverse topics as chemistry in space and organometallic synthesis. Time resolved spectroscopy and matrix isolation are techniques that still provide valuable insights after more than 50 years, and as emphasized by Houk, this will continue.

Linear free energy relationships began with the Brønsted equation, and as noted by Engberts, Kosower, and Katritzky, these will be increasingly useful, particularly as a way of systematizing the wealth of data available from physical organic chemistry. This area will be of particular utility in the pharmaceutical industry, and in the design of new materials.

Rather weak individual interactions such as hydrogen bonding magnified by cooperative effects and solvation have decisive effects in large systems, including biological organisms, and studies of these phenomena will receive increasing emphasis in both computational and experimental investigations, as noted by Roberts and Engberts. The formation of molecular assemblies may be studied by gas-phase, solution, and theoretical techniques, and the merging of these disciplines will receive increased attention in the future.

Reactive intermediates will continue to be studied, including carbocations (Olah), free radicals (Ingold), and carbenes (Nefedov). The study of free radicals, begun by Gomberg at the beginning of the Century and pursued ever since by physical organic chemists, has proven to be of increasing value in organic synthesis, biological mechanisms, spin labeling, and industrial processes, particularly polymerization.

Organometallic chemistry is a rich ground for future physical organic chemical investigations, and the state and promise of the field has been ably and extensively summarized by Yamamoto and Schwarz. Much of chemistry is about making things, and the physical organic chemist is involved in this area, in the design and constuction of unusual and theoretically interesting molecules, and also the deliberate study of molecular materials and supermolecules (Breslow, Lahav, Mukaiyama). The role of mechanistic analysis in designing new synthetic reactions will continue.

Houk traces the growth of computational and theoretical organic chemistry from the 1960's, and most of the authors confidently expect an ever-increasing emphasis on such studies. As discussed by Saveant, electrochemistry is a powerful and convenient technique that offers rich rewards, and warrants increased use, particularly in the study of electron transfer processes and nonhomogeneous kinetics.

Kosower highlights the political and economic influences on the practice of chemistry, and the need for greater sophistication in these areas for chemists. Several of the authors (Arnett, Fox) note that students trained in physical organic chemistry have favorable employment prospects in industry, as they are experienced in problem solving. Others (Arnett, Engberts) predict an increasing trend toward group, as opposed to single, investigator research.

As noted by Arnett one of the greatest contributions made by physical organic chemistry is the collection of simple qualitative theories of broad applicability such as transition state theory, Hückel's rules, the Woodward-Hoffmann rules, resonance, and hard-soft acid-base concepts. These are ultimately the product of human intellect, however much assistance is provided by large computers, sophisticated instrumentation, and diligent laboratory work.

Finally there will be the unexpected, and as Mukaiyama and others point out in the saga of the fullerenes, there are still limitless opportunities for new discovery and surprise in the area of physical organic chemistry.