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Physical organic chemistry: Quo vadis?

Jürgen Vogt and Daniel Bellus

Ciba-Geigy, Corporate Research Units, Marly and Basel, Switzerland

Biography: Daniel Bellus, born in Trnava in 1938, studied chemistry in Bratislava, where he obtained his Ph. D. on a topic dealing with polymer analogous reactions. From 1967 to 1969 he carried out postdoctoral studies at the ETH Zurich with O. Jeger and K. Schaffner in the field of organic photochemistry. In 1969 he joined Ciba-Geigy, where he is presently Head of Corporate Research Units, thus responsible world-wide for research programmes in selected areas of the chemistry of bioactive compounds, materials, and analytical science. He is the author of 85 publications and holds 48 patents. From 1980 he has lectured at the University of Fribourg (Switzerland), and received the Scientific Prize of the City of Basel (1982) and honorary doctorates from the Slovak Technical University (1991) and Comenius University in Bratislava (1992).

Jürgen Vogt, born in 1945, directs the Materials Research Department, which is one of Ciba-Geigy's Corporate Research Units. He has studied chemistry at the Technische Hochschule Darmstadt/Germany and obtained his Ph. D. in physical chemistry from the University of Basel/Switzerland with studies on the unimolecular fragmentation of organic ions. After postdoctoral work at the California Institute of Technology on ion-molecule reactions and further work on ion fragmentation mechanisms he was nominated Privatdozent at the University of Basel. In 1980 he joined Ciba-Geigy, first with the Plastics and Additives Division, later with Corporate Research, performing and coaching interdisciplinary work on polymeric materials and systems. He is author or coauthor of some 40 publications and continues to lecture at the Universities of Basel and Fribourg/Switzerland.

In the following short essay we first discuss the race into extreme specialization in the field of physical organic chemistry from our industrial point of view and its potential effect on the education of chemistry students, after which we try to give a few hints which might be worth considering in planning education and research in physical organic chemistry.

During recent years we experienced outstanding developments in all domains of physical organic chemistry. Typical of these are the extensions into the fields of organic and supramolecular chemistry, computational chemistry, biochemistry, and medicine. This development is a logical and necessary one, since in all the fields mentioned the methods and results of physical organic chemistry are needed and used for further progress on the molecular level.

The main purpose of "classical" physical organic chemistry was and still is the elucidation of reaction mechanisms and the measurement of the kinetics of the individual elementary chemical reactions. In this respect we are witnessing the development and exploitation of ever faster, more elaborate, and more sophisticated types of spectroscopy and other methods, capable of splitting even femtoseconds and recording the corresponding response of atoms and molecules. The exploration of this short-time domain is considered to belong to the realm of physics, since this experimental time window, not even allowing a sizeable fraction of a fast molecular vibration, is usually too short to really expect "chemistry" to happen. Research in this field becomes increasingly expensive and the nature of the questions to be answered gets extremely narrow. In quite a few cases methods have been developed that await their fruitful use.

Most often the overriding reason behind this development is the general tendency of institutions and authorities, which decide on and distribute research grants, to channel the research money into proposals targeting the extremes in different technologies. The myriad experiments and scientific questions which may be mastered with existing and more conventional technologies seem to be too normal and therefore not of sufficient interest.

In fact, the gap between the development and availability of highly sophisticated methods in physical organic chemistry and their actual use to tackle relevant and real problems of industry and society at large is widening. This has several consequences, some of which will be discussed subsequently.

As an example, the field of interaction of light with condensed matter is taken. Although of utmost interest in, *e.g.*, industrial photopolymer applications such as photocuring coatings and microlithography, only some limited knowledge is available on the elementary reactions occuring in photoresist formulations, leaving the total system often too complicated for a complete assessment. Methods to follow the reaction mechanisms and to quantify the kinetics of industrially used photopolymerizations are only rudimentarily developed. Additionally, due to the compexity of all the reactions running in parallel and in sequence, the amount of experimental work necessary for analysis of such complex systems is considerable.

Essentially all uses of lasers in processing of materials fall also into this category of highly complex reactions. Elegant experiments have been designed and performed involving laser spectroscopy on single molecules in the gas phase or in an inert matrix, but usually only the monomolecular information has been discussed. Practical applications of high intensity laser light mostly with the wanted non-linear effects, resulted in the majority of cases in developments on a pure trial and error method, lacking the understanding of the basic principles behind. Similarly, surface chemistry, and specifically surface photochemistry is considered as extremely complex. Examples of this are heterogeneous photocatalysis and many of the light induced surface reactions.

Consequently, it is not surprising that academia strives for more extreme and more expensive experimentation, since it seems more likely to achieve higher scientific recognition with femtosecond spectroscopy on single molecules than by tediously analyzing complex reactions. Additionally, analysis of complex systems usually requires an interdisciplinary approach, *i.e.*, the interaction of different specialists, who increasingly have difficulties to communicate because of their extreme specialization.

All these trends have, among others, two adverse consequences. One is, since large portions of research grants go into the funding of extreme experimental techniques which are also extremely expensive, less money is left for "normal" but nevertheless necessary and useful technology related research. The other effect is on the education of our present students. They get trained to be highly specialized in the extreme technologies which are not very likely to be used in everyday industrial applications (most of the students eventually end up in industrial jobs), whereas the average student's knowledge of the combined use of the more normal but readily accessible experimental methods (in organic and physical chemistry) remains rather limited.

Based on our experience and on the problems which we encounter in our daily research life in a research-oriented enterprise, we dare to point out some "normal" needs, which we think belong to the domain of physical organic chemistry. The topics listed below are of industrial importance and, judged from our admittedly subjective point of view, are presently not adequately accounted for in research and education:

- complex neutral and ionic gas phase chemistry, such as plasma chemistry;
- surface chemistry, solid-gas, such as plasma etching and coating, radiation (UV) induced surface reactions, as well as solid-liquid interfacial reactions such as wet chemistry surface modifications (plethora of work is done on surface characterization, but controlled and reproducible surface chemistry seems still exceptional);
- organic solid state chemistry (crystalline and amorphous solids, allotropes, different spectroscopic and chemical behaviour, change in morphology upon heat and radiation treatment);
- physical organic chemistry on polymers, oligomers, and polymer solutions in general and specifically in conjunction with the above mentioned topics. The resulting work has intentional overlap with polymer physics. Interesting new materials applications are expected from such interdisciplinary research;
- chemiluminescence, which usually had the nimbus of extravagance, but which in recent years has slowly matured to become extremely useful as a diagnostic tool in biomedical assays as well as in studying, *e.g.*, the aging of polymers, specifically of (thermally induced) oxidative degradation processes.

Thanks to the recent developments in physical organic chemistry practically all modern research activities in molecular science areas like chemistry, biology, and physics are heavily depending on complementary work in physical organic chemistry. This is particularly true for research and development programmes in any industry which concentrates on the design, synthesis, and production of receptor-oriented, biospecific compounds. We only can hope that also in the field of physical organic chemistry the "scientific market forces" are effective enough to prevent academic research from drifting too far away from practical needs. Retreat into the ivory tower of science driven by further specialization is not considered as beneficial for the professional careers in industry of the forthcoming generation of physical organic chemistry students.