Journal of Thermal Analysis and Calorimetry, Vol. 57 (1999) 3-6

Special Issue
on
Applied Physical Chemistry

Dedicated to ***Dr. Erwin Marti***
on the occasion of his 65th birthday

Guest Editors:
Dr. W.-D. Emmerich
Netzsch-Gerätebau GmbH, Selb, Bayern, Germany
Dr. D. Giron
Novartis Pharma AG Basel, Switzerland
Dr. U. Ch. Hofmeier
Novartis Services AG, Basel, Switzerland
Prof. Dr. H. R. Oswald
Universität Zürich, Switzerland

The Guest Editors express their gratitude to all who have contributed to this Special Issue, especially to all the authors of manuscripts covering valuable subjects of applied sciences. Many thanks are also expressed to the Editors, Mrs. J. Simon and Ms. B. Androsits, for their cooperation.
We are also thankful to all additional referees who have reacted without reluctance to our demands: Prof. F. P. Emmenegger, Fribourg; A. Geoffroy, Basel; Dr. E. Grell, Frankfurt; Prof. J.-P. E. Grolier, Clermont-Ferrand; Prof. H. E. Junginger, Leiden; Dr. I. Marison, Lausanne; Dr. M. Mutz, Basel; Prof. A. Reller, Augsburg and Dr. H. Weber, Spreitenbach.

It was a great pleasure to enlarge with this Special Volume the network of the **European Society for Applied Physical Chemistry** and to publish a number of selected contributions which were presented during the **PhandTA 3**, Symposium/Workshops on Pharmacy and Thermal Analysis, held from October 12 to 15, 1997 at Centro Stefano Franscini, Monte Verità, Ascona, Switzerland.

1418–2874/99/ $ 5.00

Akadémiai Kiadó, Budapest
Kluwer Academic Publishers, Dordrecht

Erwin Marti was born on December 27, 1932 in Basel, Switzerland.
In 1957 he enrolled at the University of Basel to study physics, chemistry and mathematics. A discussion in 1958 with Professor Werner Kuhn, then head of the Institute for Physical Chemistry was already decisive for Erwin Marti to select Physical Chemistry as his main study direction. Werner Kuhn was an excellent researcher, with a combination of extraordinary intelligence and outstanding creativity. Werner Kuhn applied molecular and thermodynamic principles to technical and biophysical projects such as distillation methods, e.g. to gain $D_2{}^{18}O$ from natural water; study of the properties of substances and materials, and especially the form and the shape of polymers and biopolymers as dispersed systems; transport and diffusion through membranes and in solids; the development and description of models for artificial kidneys, artificial muscles and the function of the swim bladder of fish.
In 1963, the thesis of Erwin Marti about the multiplication of a single concentration effect in a countercurrent system as model for the gas concentrations (CO_2, N_2, O_2 ...) in the swim bladder of fish, as well as the salt and the urea concentrations in the loop of Henle of the kidney, was accepted.
In 1966 Erwin Marti moved, after a period of 6 years for the thesis and a postdoctoral position in Basel, to a second postdoctoral position in Berkeley, University of California. Professor Harold S. Johnston, head of Physical Chemistry, was the leading scientist in unimolecular gas phase kinetics, which he applied to smog and ozone chemistry. Prof. Johnston's group in Berkeley were honored in 1995 by the award of the Nobel Prize to former students Prof. P. Crutzen, Prof. M. J. Molina and Prof. F. S. Rowland for their work on ozone.
Erwin Marti married Alice Stieger in 1961. Dominik, born in 1962, today a medical doctor, and Barbara, born in 1964, a children's nurse, were with the parents in Berkeley. Florian, today a financial manager, was born in 1970. The daughter Barbara and Pierre Siegrist have two children, Anna and David.
Erwin Marti decided with his family to go back to Switzerland and in 1968 he accepted a position in the Central Research Department of the J. R. Geigy AG in Basel. He did not change his position as a physicochemist, not even as a consequence of the two mergers, into Ciba-Geigy Ltd. and into Novartis Ltd. What could be regarded as a fairly straight-forward position, developed under his activity into a highly complex project management in the areas of research, development, and production of active substances. He was always involved in laboratory work and was leader of a large number of projects. The sectors of the chemicals produced at the Ciba-Geigy Ltd. were extremely broad, ranging from pharmaceutical and agrochemical substances to additives, polymers, pigments, dyestuffs and chemicals. As an example, a fine crystalline powder produced in a Geigy factory turned into heavy lumps during production and under the storage conditions. Erwin Marti wrote to the head of production one year before the problems of lumping started, that the substance would create difficulties in the ball mill grinder. The investigations he started in 1968 for the purity determination by DSC, and of the interrelation of eutectic purity and phase diagrams for organic multicomponent systems, were the scientific base to the necessary actions which had to be taken to solve this specific problem of physical instability. Dr. Ernst Keller, head of the Central Research Department, was extremely pleased with the measures taken for this production unit and promoted Erwin Marti to the position of a senior chemist.
In 1983, Erwin Marti made a proposal concerning the destruction of dioxin-containing waste from Seveso. He became project leader of the team 'Thermokinetics and Flue Gas Analysis' within the governmental Commission of Experts. The complexity of the project demanded knowledge in areas such as unimolecular gas phase kinetics and testing of an industrial waste incinerator at temperatures much higher than 1200°C. The development

of a fast analysis of the stack gases for dioxins, involving the sampling, extraction of the adsorption filter (5 mg of active carbon), the introduction of isotopes for the calibration and finally GC-MS measurements on a detection limit in the pg range for 2,3,7,8-TCDD/m^3 flue gas, was a critical step of the project. The second main achievement in this project was the introduction of 2,4,8- trichlorodibenzofuran for test burning in the rotary kiln as reference substance. In the laboratory it was possible to measure the decomposition for the reference substance as well as for 2,3,7,8-TCDD in small sample sizes and transfer these findings from the laboratory together with the results from test incineration as an estimation of the destruction efficiency of 2,3,7,8-TCDD in the rotary kiln.

The solid state characterization of crystalline and amorphous substances and the investigations of the corn size stability of crystalline powder beds has been one of his research activities for more than 30 years. The development of an in-process control method for the clearance of production batches, with respect to a demanded stable crystal modification in an industrial process running day and night, is an example in the quality control area. The development of several vapor and partial pressure methods for a broad application to substance characterization, mainly for the estimation of the toxicological actions of chemical compounds over the gas phase, as well as for the design of physical processes, made his laboratory an exceptional one. Another area of interest was the development of different procedures in the application of high sensitivity isothermal calorimetry in the study of the chemical and physical stability of drug substances and drug products as well as for agrochemical formulations. The introduction of kinetic procedures by means of scanning and isothermal DSC and thermobalance measurements and the evaluation of the generated data, for the determination of the physical and chemical stability of active substances also in form of hydrates and solvates within the different phases in the research and development, required special attention.

Erwin Marti started in the Physics Department on May 6, 1968. The single coworker, the late Oskar Heiber, introduced Erwin Marti to the laboratory work. One important instrument, a DSC, was available in this laboratory. This instrument opened many activities for our group within the areas of thermal analysis. The instrument was handed over with a report and the statement that quantitative measurements could not be achieved, however, important qualitative studies about the polymorphism of chemical substances should be possible. This was certainly a challenge for the newcomer. The procedures necessary for a quantitative purity determination had been elaborated carefully. The development of a calculation and linearization procedure for melting curves allowed the determination of the absolute eutectic purity even for very coarse crystals and also for heavily distorted melting curves. The results of these investigations were presented in Davos in 1971 at the 3rd ICTA and evoked interesting discussions among the experts. The 3rd ICTA was the beginning of many activities at conferences and in societies for all the members of Marti's group.

In 1974 the study of polymorphs and the determination of stability regions on a quantitative thermodynamic base had been undertaken. The Gibbs free energy functions were calculated using a set of thermodynamic data, namely the melting temperatures and the enthalpies of fusion. Important were the measurement of the molar heat capacities for the polymorphs under investigation as well as for the molten phase common to all of the polymorphs of a substance and therefore selected in our laboratory as an ideal reference state. Erwin Marti's approach was different from that of other research groups, namely to elaborate absolute stability regions by a calculation of the thermodynamic transformation temperature and afterwards to verify the stability regions by means of selected kinetic investigations or by additional physicochemical measurements such as solubility, X-ray diffraction and vapor pressure.

Today the field of thermal analysis has broadened extensively with methods such as titration calorimetry for binding studies, scanning microcalorimetry and temperature scanned UV absorbance for denaturation and stability studies of biomolecules. Hyphenated instruments such as TG-MS, DSC-GC-MS, TG-FTIR, Raman and FTIR microscopy with a hot-stage platform, powder X-ray diffraction combined with a heating device, enable the combination of thermodynamic information with spectroscopic molecular characterization. Thermodynamics, calorimetry, thermal analysis, kinetic mechanisms, reactivity, spectroscopy, electron microscopy, micro-sensor technology and others are integrated in an appropriate way by the term **Applied Physical Chemistry**.

On his first day at J. R. Geigy AG a letter was on the desk of Erwin Marti from the head of the pharma division with the request to give support in connection with a patent conflict. A clear scientific basis is the best way to deal with such problems. It could be revealed by an interesting physicochemical study that Geigy was outside the claims of the plaintiff. This first contact with the patent world opened new aspects. A number of new chemical entities were found over the years and in most of the cases the research work and the possibility of patenting were proposed by Erwin Marti.

The scientific societies in which he and his coworkers are integrated, are the basis of a worldwide network covering the subject of Applied Physical Chemistry. Such a situation is decisive in an industrial research position with the great variety of chemical and physical projects and problems to be investigated and to be solved.

In 1974 Erwin Marti received a letter from Professor H. Lehmann, the first president of GEFTA (Gesellschaft für Thermische Analyse, Germany) with the invitation to join this society as a member together with other Swiss scientists. He wrote back that the Swiss collegues, especially Professor Oswald, were in favor of a Swiss society, due to the multilanguage situation in Switzerland. The Swiss Society for Thermal Analysis and Calorimetry (STK) was founded in 1975, with Professor Oswald as the first president. Erwin Marti followed him in 1979 and he is in this position to this day.

In 1992, a new society was founded within a nucleus of scientific colleagues of the president of the STK, the European Society for Applied Physical Chemistry, with the logo *eurostar-science*. The board of this society organizes conferences with an emphasis on specific subjects, similar to the Gordon Research Conferences, following the ideas of the late Dr. Paul Rhyner, the long-time president of the 'Schweizerische Chemiker Verband' and former head of the Central Research of the Ciba-Geigy AG. The habit of life-long learning is a challenge for the activities within these scientific societies.

The two societies, the STK and *eurostar-science,* will convene together in the Pharmazentrum in Basel in the last week in September 2000. The Swiss Society will celebrate its 25th anniversary, and the board of *eurostar-science* will organize the PhandTA 5. All these activities of Erwin Marti in the chemical industry as well as in the function as president in these two scientific societies, could only be achieved with the support from the three chemical companies: Geigy, Ciba-Geigy and Novartis. Also the valuable support from many instrumental manufacturers has to be mentioned. Another important factor was the friendly support of different groups of coworkers and colleagues from industries and universities. The generosity of his family, especially of his wife, Alice, was a prerequisite for all these scientific activities.

The scientific situation at universities and institutes, and also in the chemical and pharmaceutical industries has changed drastically since 1968, however, further changes can be foreseen for the near future. The question is who will take over the work of Erwin Marti for the next generation? Time will solve this open question.