

LETTERS OF WELCOME

The following letters were received by the Editor on the occasion of the founding of the new journal.

Palo Alto, California

30 September, 1986

It is fine that you are to serve as the Editor of the new *Journal of Mathematical Chemistry*.

I believe that there is need for such a journal. During the last 60 years, the number of aspects of chemistry that can be treated in a significant way by applying mathematics has been increasing rapidly.

For many years, beginning in 1926, I myself applied quantum mechanics to chemical problems. Some of the applications involved rather unusual mathematical functions, such as the Gegenbauer functions. Even during the last two years I have been applying mathematics to a chemical problem, the problem of the nature of the electronic structure of metals, by means of a rather complicated resonating-valence-bond treatment, a statistical treatment.

I look forward to seeing the first issue of the Journal.

Sincerely,

Linus Pauling

Nobel Prize in Chemistry 1954

Nobel Prize in Peace 1963

Zürich, Switzerland

30 September, 1986

I am flattered by your invitation to write a letter to support the new *Journal of Mathematical Chemistry*. As both a layman and an amateur in this field, and to boot one who is presently very much occupied with the celebration of his 80th birthday, I feel somewhat overcharged by this task. Nevertheless, I would like to make the following brief comments.

It is now some 200 years since Immanuel Kant averred that "in any branch of study of the natural world, the amount of actual science contained therein is directly proportional to the amount of mathematics

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used". On the basis of this criterion, it is hardly surprising that he drew the conclusion that "chemistry can under no circumstances be regarded as a science".

With the development of what is known as structural theory by early workers such as Butlerov, Couper and Kekulé, came the introduction of the structural formula. Although these pioneers did not recognize that the structural formula they introduced was a mathematical object, namely a chemical graph, it was not long before a mathematician pointed this out. Arthur Cayley first made use of chemical trees in his calculation of the numbers of constitutional isomers in homologous series such as the alkanes. This work was to lay the foundations of modern combinatorial theory. It was George Pólya's interest in isomer enumeration problems that led him to his famous Enumeration Theorem.

After the establishment of structural theory, the symmetry of molecules began to play an increasingly important role. The great pioneers of this field, namely Jacobus van't Hoff and Achilles Le Bel in organic stereochemistry and Alfred Werner in inorganic stereochemistry, did not recognize that they were making use of a mathematical tool. Group theory has since proved invaluable in the study of numerous problems associated with stereochemistry.

The gradual evolution of physical chemistry has also been responsible for the introduction of manifold mathematical concepts into the realm of chemistry. Examples include the use of calculus to treat problems in chemical thermodynamics and kinetics, linear algebra for quantum-chemical calculations, group theory for molecular spectroscopy, computer science for computations in molecular mechanics, structural analysis, the design of synthesis routes, and the analysis of reaction pathways.

It is thus very evident that progress in chemistry will depend to an ever-increasing extent on the application of relevant mathematics. Accordingly, I am very glad to be able to support the initiative taken in founding this new journal. From the standpoint of Kant, modern chemistry already includes more than enough mathematics to be classified as a respectable science. I am convinced that the new journal will continue in the tradition of showing how vitally important mathematics will be in the future development of chemistry.

With best wishes,

Vladimir Prelog

Nobel Prize in Chemistry 1975

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Washington, D.C.

10 October, 1986

I was pleased to learn that a *Journal of Mathematical Chemistry* is about to be established. The establishment of this *Journal* implies that mathematical chemistry is being recognized as a valuable context in which to categorize a broad range of activities that play a fundamental role in the progress of chemical science. A particular virtue of drawing together the great variety of theoretical approaches to chemistry is the potential for sharing deeper insights into the applicability and utility of commonly used mathematical techniques such as Fourier transform theory, probability theory, the mathematics of quantum theory, and the theory of differential equations.

It is my hope that the collection of forthcoming articles in the *Journal of Mathematical Chemistry* will also serve to emphasize the important role of a process that I and others call "bridging", which arises in applications of mathematical theory. Bridging concerns the modifications of theory and the treatment of experimental data that permit theory and experiment to be suitably combined. Insightful modifications and adjustments often make the difference between the success or failure of a theoretical approach to a problem, and they are often as much a part of a new theoretical development as the purely mathematical manipulations.

My interest in the applications of mathematics to other fields of science arose in my student days. In addition to the joy of discovery and new understanding, the attraction of this activity has been the opportunity that theory provides for general comprehension, deep insights into the nature of fundamental processes and quantitative description.

The value of mathematics to chemistry requires no acknowledgement. Although mathematical chemistry has not generally been referred to under such a title, it has a long history with much continuing interest. Many areas of chemical science are replete with such examples, e.g. quantum chemistry, structural chemistry, reaction dynamics and mechanisms, chemical thermodynamics and statistical mechanics.

Mathematical chemistry provides the framework and broad foundation on which chemical science proceeds. There is much activity and interest in the various disciplines that comprise this area of investigation, and therefore the establishment of the *Journal of Mathematical Chemistry* is well-justified with the potential for catalyzing the enhancement of this important aspect of chemistry.

With all best wishes for the future,

Sincerely yours,

Jerome Karle

Nobel Prize in Chemistry 1985