

EDITORIAL FOREWORD

Mathematics and chemistry make excellent partners. Cross-fertilization of mathematical theory with chemical concepts has been responsible for the growth of major areas of chemistry over the past two centuries. The ongoing mathematization of chemistry shows no sign of abating and has in fact gained significantly in pace in recent years. This is a process we welcome and one that we view as a natural concomitant of the evolution of chemistry as a whole. We believe that the future vitality of chemistry is very much linked to the cultivation of new mathematical models and techniques which can be used to characterize chemical systems. Because of our belief in the decisive role of mathematics in the future of chemistry, we felt the time had come to found a new journal devoted to mathematical chemistry. There are several reasons for the appearance of the journal at the present time. There is certainly the burgeoning growth of the field already alluded to. This growth has brought in its wake a number of problems: overloaded journals, long publication times, insufficient choice of appropriate journals, less than optimal refereeing, and perhaps a certain amount of resentment from the chemical community at large of the unruly new *enfant terrible* that now goes under the name of mathematical chemistry.

Our new journal is intended as a natural home for papers in the general area of mathematical chemistry. This raises the very natural question of what we understand by the term *mathematical chemistry*, at least for the purposes of this journal. Perhaps we might start by saying what mathematical chemistry is not. It is certainly not the routine application of well-trying and well-worn mathematical techniques to problems of a chemical nature. A goodly portion of theoretical chemistry, including much of quantum chemistry and the various types of mechanics (molecular, quantum, and statistical), tend to fall in this domain and are thereby eliminated from our ambit. Computational chemistry is also excluded; papers in which the details of more or less standard computations are described are not suitable for this journal. Mathematical chemistry concerns itself primarily with the *novel* application of mathematical methods in the chemical realm. The novelty is commonly expressed in one of two ways, viz. (i) the development of new chemical theory, and (ii) the development of new mathematical approaches which enable us to gain insights into or to solve problems of chemical interest.

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The type of mathematics employed is immaterial; its novelty in respect of the chemical problem under consideration is all important as far as the journal is concerned. Some spectacular successes were achieved with the introduction of mathematical methods in the nineteenth century. Mention need only be made of the tremendous impact of the calculus in the field of chemical thermodynamics, or of statistics and information theory in statistical mechanics. In the present century, vector and matrix algebra has been vital in the development of quantum chemistry. The now wide acceptance of group theory is but a reflection of its power and elegance in dealing with problems relating to molecular symmetry. Very recently, fields such as combinatorics, graph theory, and topology have come to the fore and again have been used to tackle a very broad span of chemical problems. All of these branches of mathematics, and many others, have been and are still being applied in chemistry in new and exciting ways. Papers covering any of these areas will be appropriate for the new journal.

All papers submitted to the new journal are subject to peer review by at least two referees. Papers in the following four categories can be accepted for publication: (i) full research papers; (ii) author or general review papers; (iii) research notes (up to twenty typed pages in total); (iv) research letters (up to six typed pages). As reviews are likely to be of value to most of our readers, such papers will be encouraged. Endeavor will be made to secure timely reviews from as many different areas of mathematical chemistry as possible, and it is hoped we may succeed in having one review in each issue of the journal. For the present, the journal is planned to appear quarterly, though it is anticipated that the frequency of appearance will be stepped up to meet any rising need.

It would not be possible to embark upon an enterprise of this magnitude without the assistance and support of a large number of different people. I should therefore like to take this opportunity of thanking all of them publicly here. Specific mention is made of my Editorial Advisory Board members, who have agreed to serve for an initial five-year term and who will have the task of advising on what is appropriate for the new journal and of deciding on any new initiatives we may wish to try out. I am greatly indebted to the three distinguished authors who sent letters of welcome to me for the first issue of the journal; their gracious support of our new venture is highly appreciated. In addition to these great pioneers of mathematical chemistry, thanks are also due to the many currently very active authors who mailed their papers to me for this and other early issues of the journal, without knowing precisely what form the journal would take. Finally, I should like to express my gratitude to the publishers of the journal, the J.C. Baltzer Scientific Publishing Company of Basel, Switzerland. Their faith in the project from its inception, their unfailing encouragement and support, and their courtesy and forbearance in coping with problems have been exemplary. The unstinting support of all of these and others has made the task of establishing this new journal a rich and rewarding experience, and augers well for the future success of our journal.

Dennis H. Rouvray
Editor