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# Partial Order in Environmental Sciences and Chemistry

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(Editors)

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With 140 Figures and 50 Tables

Springer

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# Preface

When you edit a book, the editors should ask themselves, why are we doing this and whom are we doing this for? To whom could this book be valuable as a source of information and possibly inspiration and of course are there other books with similar topics on the market? Indeed the mathematical structure 'partial order' is explained in many mathematical textbooks, which require different degrees of mathematical skills to comprehend. Thus, as far as we can tell, all these books are dedicated directly towards mathematician working in the area of Discrete Mathematics and Theoretical Informatics. Although partial order is very well known in quantum mechanics, especially within the context of Young-diagrams, literature stressing the application aspect of partial order seems to be not available. However, an increasing number of publications in scientific journals have in recent years appeared, applying partial order to various fields of chemistry and environmental sciences. A recent summary can be found in a special issue of the journal Match - Commun.Math.Comput. Chem. 2000, edited by Klein and Brickmann. However, we believe that this journal possibly is too specific and as such it may not reach scientists actually applying partial order in various fields of research. Hence, we dared to initiate the editing of this book in order to address a broader audience and we were happy to convincing distinguished scientists working with different aspects of partial order theory to contribute to this book. We are indeed indebted to all of them.

What is a partial order? A general explanation can be found just in the first chapters of this book and according to the different application aspects, correspondingly adopted definitions can be found in many other chapters; however, it might be useful briefly to explain the concept here by a simple example. Thus, if a chemical is toxic and is bioaccumulating then obviously the chemical may exert an environmental risk. If there are two other chemicals, one exhibiting a lower toxicity but a higher bioaccumulation potential and another with a much higher toxicity but a lower bioaccumulation potential, we may have a problem to assess their individual environmental risks. This kind of problems can be analyzed with partial order. The only mathematical operation needed is the comparison, i.e. is a larger or smaller than b. Hence, partial order in its various application aspects is the science of comparisons! Comparisons of chemical properties, comparisons of environmental systems, and even comparisons of strategies or management options are all topic that advantageously may be analyzed using partial order theory. Our objective with this book is to demonstrate how to use partial order in the field of pure chemistry, in substance prop-

erty estimations, and in environmental sciences. Some chapters will show how partial order can be applied in field monitoring studies, in deriving decisions and in judging the quality of databases in the context of environmental systems and chemistry. The charming aspect of partial order is just that by comparison we learn something about the objects, which are to be compared!

Most of the readers will probably be trained within differential calculus, with linear algebra, or with statistics. All the mathematical operations needed in these disciplines are by far more complex than that single one needed in partial order. The point is that operating without numbers may appear somewhat strange. The book aims to reduce this uncomfortable strange feeling.

Thus, we hope that this book will broaden the circle of scientists, which find partial order as a useful tool for their work. The theoretical and practical aspects of partial order are discussed in, e.g., the INDO-US-workshop on Mathematical Chemistry, a series of scientific symposia initialized by Basak and Sinha, 1998, and in specific workshops about partial order in chemistry and environmental systems. We urge scientist, newcomers as well as established partial order users to contribute to these workshops, contacts can be found by our E-Mail-addresses (brg@igb-Berlin.de or brg_home@t-online.de (Brueggemann) or LC@AwarenessCenter.dk (Carlsen)).

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