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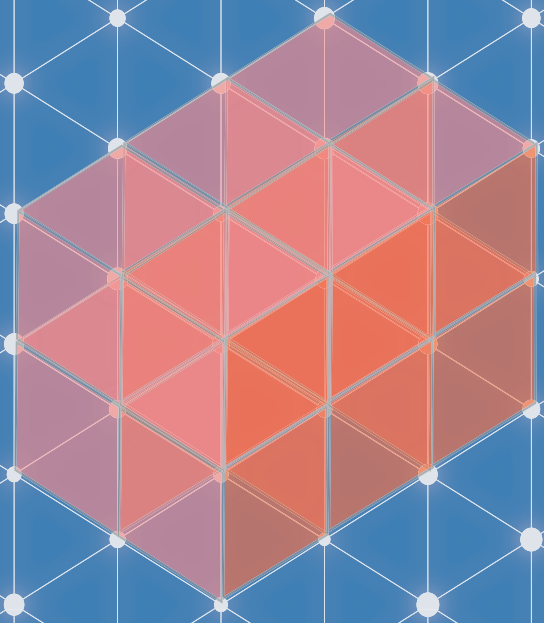
AN INTRODUCTION TO TENSOR ANALYSIS

Bipin Singh Koranga and Sanjay Kumar Padaliya



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AN INTRODUCTION TO TENSOR ANALYSIS

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River Publishers

Published, sold and distributed by:
River Publishers
Alsbjergvej 10
9260 Gistrup
Denmark

www.riverpublishers.com

ISBN: 978-87-7022-581-6 (Hardback)
978-87-7022-580-9 (Ebook)

About the Authors

This book presents basic introduction of tensors with an emphasis on the understanding of the fundamentals. It develops an appreciation of the tensor application in both undergraduate and post graduate students of Physics and Mathematics.

Bipin Singh Koranga is a graduate from Kumaun University, Nainital. He has been with the Theoretical Physics Group, IIT Bombay since 2006 and received the Ph.D. degree in Physics (Neutrino Masses and Mixings) from the Indian Institute of Technology Bombay in 2007. He has been teaching basic courses in Physics and Mathematical Physics at the graduate level for the last 12 years. His research interests include the origin of universe, Physics beyond the standard model, theoretical nuclear Physics, quantum mechanical neutrino oscillation and few topics related to astrology. He has published over 42 scientific papers in various International Journals. His present research interest includes the neutrino mass models and related phenomenology.

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AN INTRODUCTION TO TENSOR ANALYSIS

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The subject of Tensor Analysis deals with the problem of the formulation of the relation between various entities in forms which remain invariant when we pass from one system of coordinates to another. The invariant form of equation is necessarily related to the possible system of coordinates with reference to which the equation remains invariant. The primary purpose of this book is the study of the invariance form of equation relative to the totally of the rectangular co-ordinate system in the three-dimensional Euclidean space. We start with the consideration of the way the sets representing various entities are transformed when we pass from one system of rectangular co-ordinates to another. A Tensor may be a physical entity that can be described as a Tensor only with respect to the manner of its representation by means of multi-suffix sets associated with different system of axes such that the sets associated with different system of co-ordinate obey the transformation law for Tensor. We have employed suffix notation for tensors of any order, we could also employ single letter such A,B to denote Tensors.

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Editor—Acquisitions: Sharel Simon
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ISBN: 978-93-534-3837-1

eISBN: 978-93-539-4143-7

First Impression

Published by Pearson India Education Services Pvt. Ltd, CIN: U72200TN2005PTC057128.

Head Office:15th Floor, Tower–B, World Trade Tower, Plot No. 1, Block–C, Sector–16, Noida 201 301, Uttar Pradesh, India.
Registered Office: The HIVE, 3rd Floor, Metro zone, No 44, Pilliayar Koil Street, Jawaharlal Nehru Road, Anna Nagar, Chennai, Tamil Nadu 600040.
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Ajeet Jha is an Assistant Professor in History at Kirori Mal College, University of Delhi. He obtained his Post-Graduate and PhD degree from the Department of History, University of Delhi. He has been a dedicated teacher in addition to his relentlessly pursued research, which resulted in publication of his articles in reputed journals and proceedings. He has recently co-authored a book, titled *Changing Complexions of Delhi: A Study of Jhuggi-Jhopadi Clusters and Cultural Transition*, which was a part of Delhi University Innovation Project. His other areas of interest include Religion, Regional History and Culture.

Chemical Science Review and Letters
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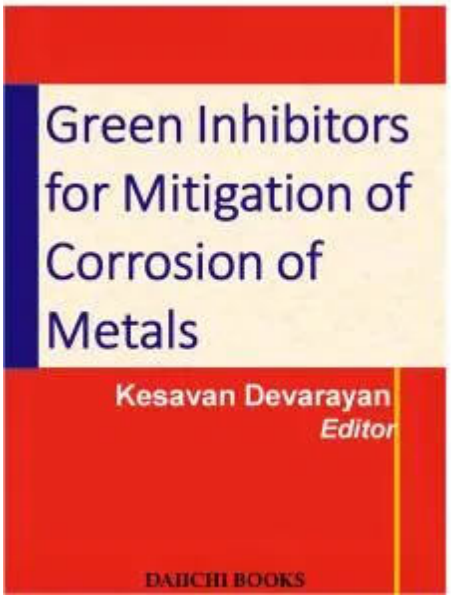
Green Inhibitors for Mitigation of Corrosion of Metals



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Author : Dr. Kesavan Devarayan (*Editor*)

ISBN : 978-81-944270-3-2

Publisher : Daiichi Books, Chemical Science Review and Letters

Language : English

Pages : 130

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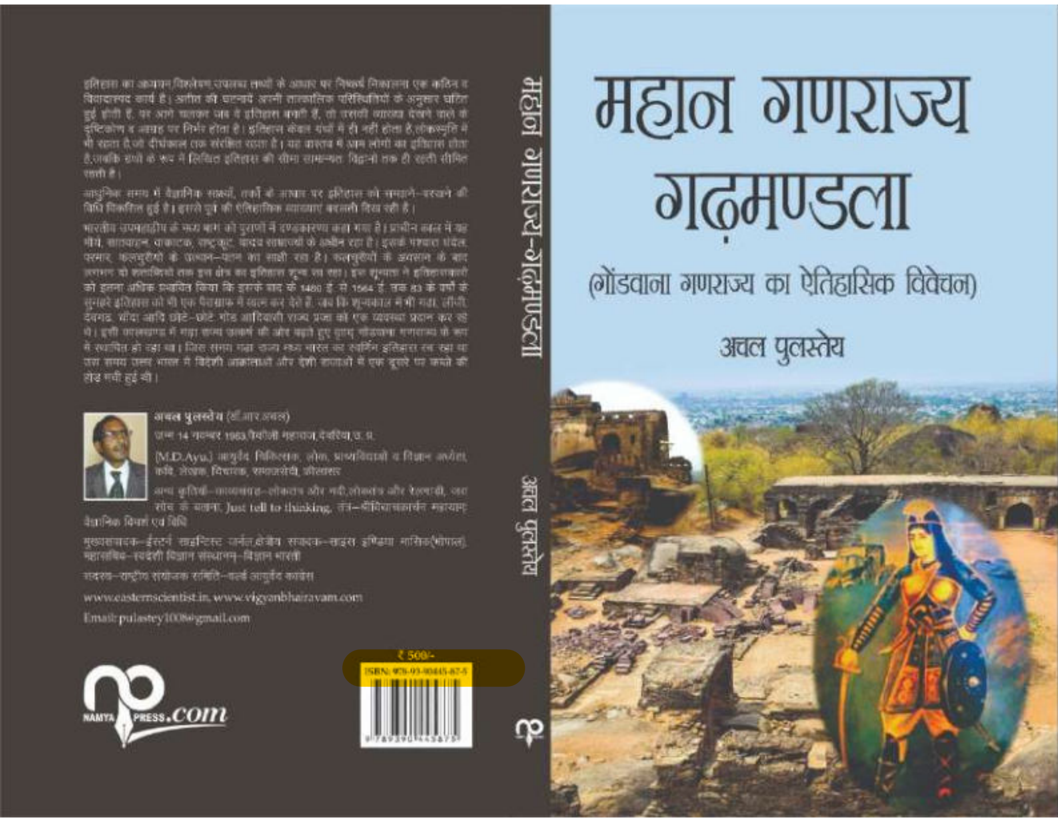

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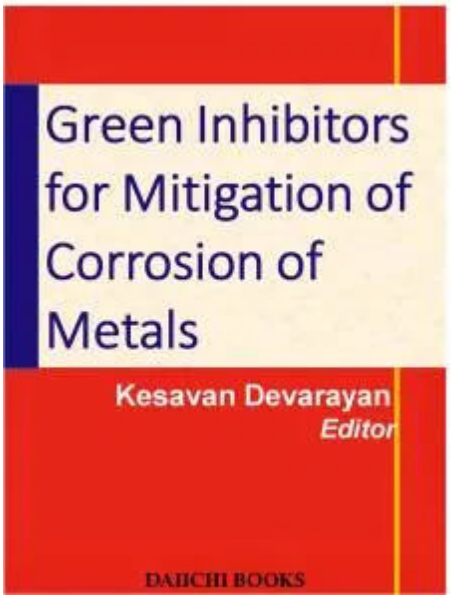

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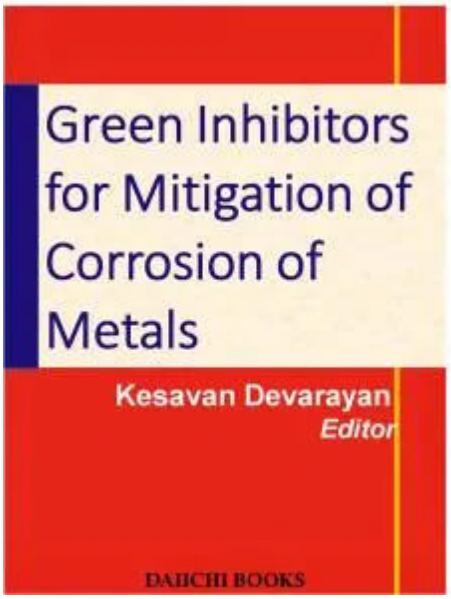

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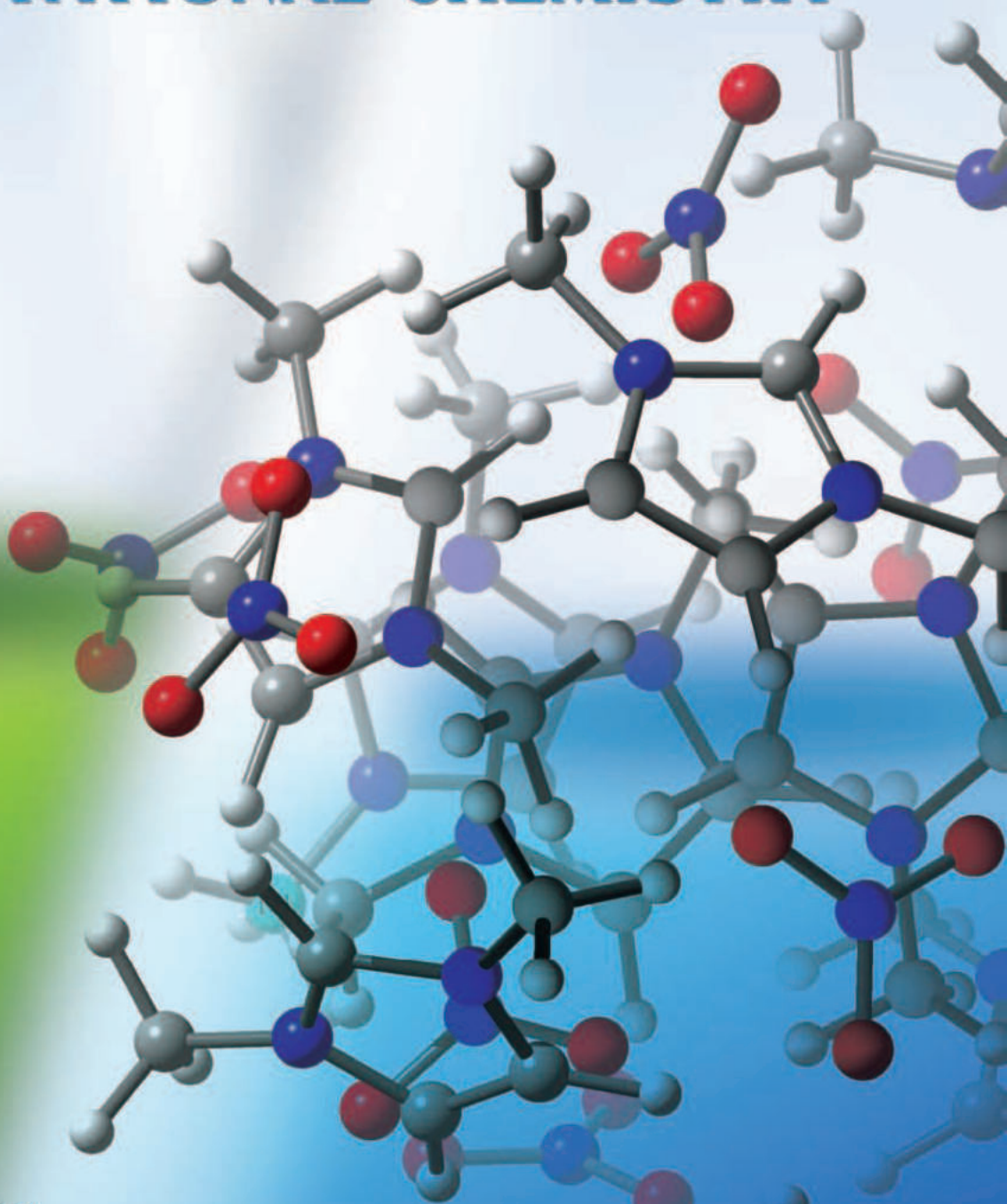
FRONTIERS IN COMPUTATIONAL CHEMISTRY



Editors:
Zaheer Ul-Haq
Angela K. Wilson

Bentham Books

Frontiers in Computational Chemistry

Volume # 5.

Editors: Zaheer Ul-Haq and Angela K. Wilson

ISSN (Online): 2352-9458

ISSN (Print): 2352-944X

ISBN (Online): 978-981-14-5779-1

ISBN (Print): 978-981-14-5777-7

ISBN (Paperback): 978-981-14-5778-4

CONTENTS

PREFACE

Computational chemistry is an important partner to experiment in understanding a very broad range of chemical problems, providing insight not possible or not easily possible to obtain via experiment, and enabling a greater understanding of experiment when it is possible. The span of computational chemistry approaches in terms of both method and applicability is significant – with methods including electronic structure calculations (*e.g.*, density functional theory (DFT)) and free energy relationships (*e.g.*, QSAR, QSPR), with applications spanning from in-depth description of the spectroscopic properties of the smallest of atoms and molecules to the design of new molecules and materials in medicine.

The focus of ***Frontiers in Computational Chemistry*** is on the application of computational chemistry approaches to biological and organic processes.

In this fifth volume, the six chapters address a diversity of topics including:

Chapter 1 "**Recent Advances and Role of Computational Chemistry in Drug Designing and Development on Viral Diseases**" Amit Lochab, Rakhi Thareja, Reena Saxena, Sangeeta D. Gadre.

This chapter outlines a number of approaches that are commonly used in drug design, including structural-based and ligand-based computational strategies, and the role of quantum mechanics and molecular mechanics. A brief overview of how these methods have been utilized in the development of drugs against viral disease, addressing ebola, zika, hepatitis C, and coronavirus is provided.

Chapter 2 "**Molecular Modeling Applied to Design of Cysteine Protease Inhibitors – A Powerful Tool for the Identification of Hit Compounds Against Neglected Tropical Diseases**" Igor José dos Santos Nascimento, Thiago Mendonça de Aquino, Paulo Fernando da Silva Santos-Júnior, João Xavier de Araújo-Júnior, and Edeildo Ferreira da Silva-Júnior.

The impact and importance of computational chemistry in drug development is significant. However, the drug discovery process is truly a fine art, with numerous methods and strategies available. In this chapter, the authors consider a number of different molecular modeling techniques, and demonstrate their use in the development of cysteine protease inhibitors. Cysteine proteases are known to play important roles from growth and development of plants to bone development in humans and animals. In this study, the design of cysteine protease inhibitors against a number of tropical diseases is considered.

Chapter 3 "**Application of Systems Biology Methods in Understanding the Molecular Mechanism of Signalling Pathways in the Eukaryotic System**", Aditya Rao S.J. and M. Paramesha.

Signalling pathways are critical cascades of reactions that can impact metabolic functions from cell division to cell death. Understanding the underlying mechanisms of signalling pathways is critical, as this can provide insight about how abnormalities can impact the activation or deactivation of signalling events. The authors provide an overview of computational routes that can be used to understand signalling path mechanisms, including systems biology and data mining. Wnt signalling pathways are the focus of this chapter due to their role in growth to cancer.

Chapter 4 "**Implementation of the Molecular Electrostatic Potential over GPUs: Large Systems as Main Target**" J. César Cruz, Ponciano García-Gutierrez, Rafael A. Zubillaga, Rubicelia Vargas and Jorge Garza.

Electrostatic interactions are vital to non-covalent interactions which are prevalent in biological systems. A very useful means to gain insight about these electrostatic interactions is via the molecular electrostatic potential (MEP). MEP is generated using quantum mechanical methods, which represents a significant computational challenge for all but the smallest of molecules. This chapter provides two routes to extend the utility of MEP to larger molecules, utilizing graphical processing units (GPUs) to generate the MEP. The theoretical details are provided, as are a number of useful examples of the application of the methods.

Chapter 5 "**Molecular Electron Density Theory: A New Theoretical Outlook on Organic Chemistry**" Luis R. Domingo, Nivedita Acharjee.

This chapter highlights molecular electron density theory (MEDT), which was introduced by the co-author, Luis Domingo, in 2015. MEDT is based upon the philosophy that changes in electron density rather than molecular orbital interactions drive molecular reactions. The authors discuss a broad range of quantum mechanical principles and approaches that are a part of MEDT and facilitate the understanding of molecular interactions and reactions. The authors provide a long list of reactions, and conclusions that can be drawn from MEDT about these reactions.

Chapter 6 "**Frontier Molecular Orbital Approach to the Cycloaddition Reactions**", Anjandeep Kaur.

Cycloaddition reactions, more specifically, 1,3-dipolar cycloaddition reactions, play a critical role from drug discovery to materials design. Controlling the regioselectivity, enantioselectivity, and diastereoselectivity of these reactions is a major challenge. In this chapter, the reactivity and selectivity of a wide variety of 1,3-dipolar cycloaddition reactions is overviewed. A Frontier Molecular Orbital (FMO) approach is considered.

We hope that the readers will find these reviews to be valuable, and that they may inspire trigger further research in the field. We are grateful for the timely efforts made by the editorial personnel, especially Ms. Mariam Mehdi (Assistant Manager Publications), Mr. Obaid Sadiq (Manager Bentham Books), and Mr. Mahmood Alam (Director Publications) at Bentham Science Publishers.

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CHAPTER 1

Recent Advances and Role of Computational Chemistry in Drug Designing and Development on Viral Diseases

Amit Lochab[1], Rakhi Thareja[2], Sangeeta D. Gadre[3] and Reena Saxena[1,*]

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Abstract: The growing number of contagious viral diseases among different geographic regions has become a threat to human health and the economy on a global scale. Various viral epidemics in the past have caused huge casualties due to lack of effective vaccine, the recent outbreak of COVID-19 is a good example of it. Drug designing and development is a lengthy, tedious and expensive process that is always associated with a high level of uncertainty as the success rate of their approval as a drug is very low. Computer-aided drug designing by utilizing *in silico* methods has shown prominent ways to develop novel drugs in a cost-efficient manner and has evolved as a rescue in the past few years. Interestingly, the highest FDA approval reached a maximum (59 drugs) in 2018 for which a lot of credit goes to the successful development of computational chemistry tools for drug designing in the last two decades. These methods provide better chances of getting hit compounds in a far more accurate and faster way. Drug designing is a cyclic optimization process that involves various steps like creating a molecule, selecting the target for this molecule, analysing the binding pattern and estimating the pharmacokinetics of the molecule. The final development of a drug candidate is cumulative of positive results obtained in each aforementioned step. Various computational techniques/approaches such as molecular dynamic studies, homology modelling, ligand docking, pharmacophore modelling and QSAR can be utilized in each phase of the drug discovery cycle. In this chapter, we aim to highlight the recent advances that have taken place in developing tools and methodologies that lead to *in silico* preparation of novel drugs against various viral infections like Ebola, Zika, Hepatitis C and Coronavirus.

Keywords: Computational chemistry, Homology modeling, *In Silico*, Ligand-based drug designing, Ligand docking, Multi target drug designing, Pharmacophore modeling, Protein target, Quantum mechanics, Structure-based drug designing, Viral infection, Virtual screening.

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Suraj Kumar Singh, Shruti Kanga, and Varun Narayan Mishra

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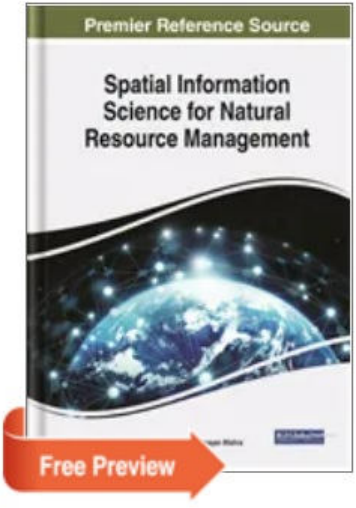

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Release Date: June, 2020 | Copyright: © 2020 | Pages: 355

DOI: 10.4018/978-1-7998-5027-4

ISBN13: 9781799850274 | ISBN10: 1799850277 | EISBN13: 9781799850281 | ISBN13 Softcover: 9781799851547

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Chapter 14
Geomorphic Changes Related to Anthropogenic Interference Along the Ganga River From Rishikesh to Haridwar, Uttarakhand, India:
Geomorphic Response of the Ganga to Tehri Dam

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DOI: 10.4018/978-1-7998-5027-4.ch014