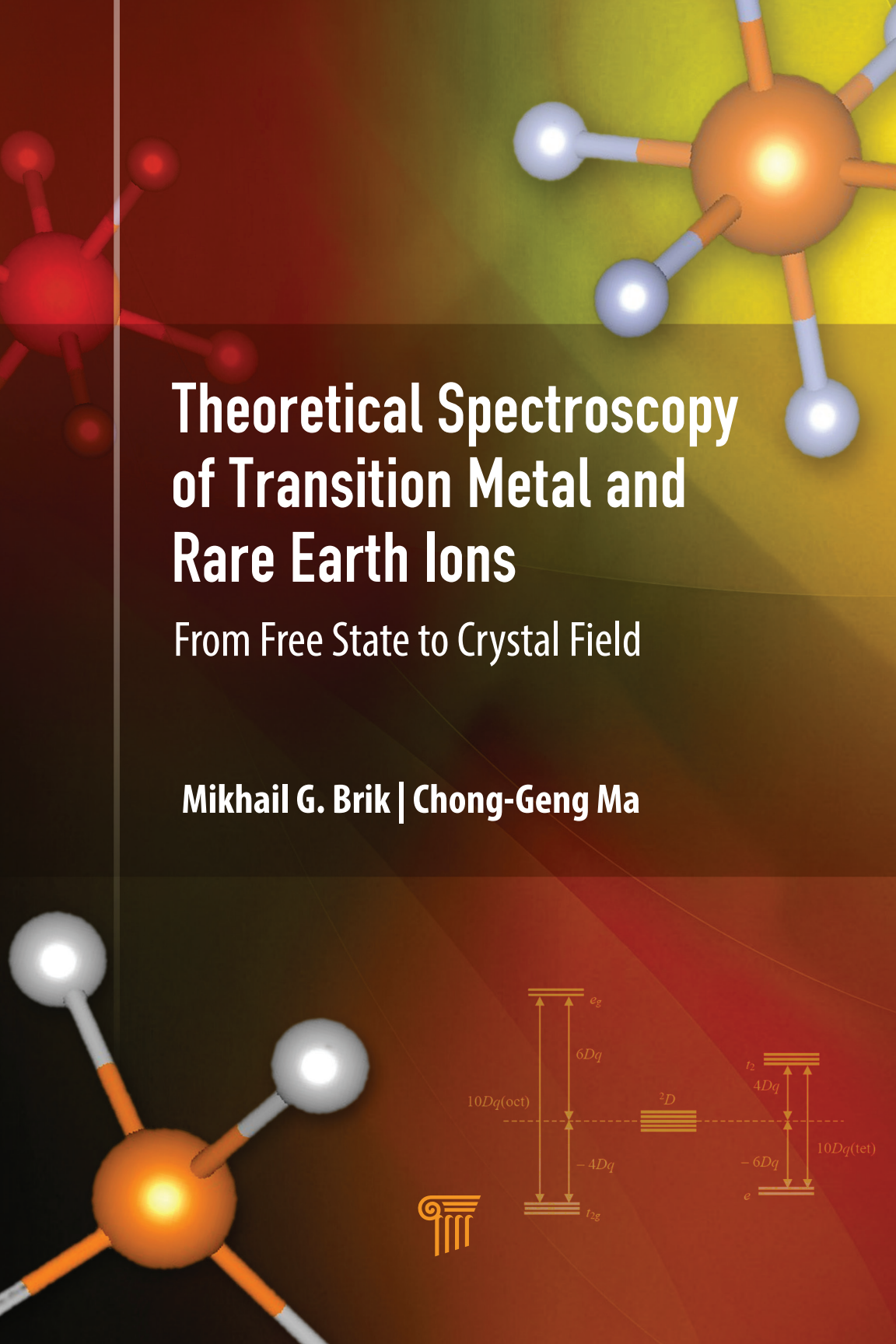
# Theoretical Spectroscopy of Transition Metal and Rare Earth Ions

## From Free State to Crystal Field

**Mikhail G. Brik | Chong-Geng Ma**



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# Preface

In the life of every scientist, there was a time of a start of the career ("once upon a time…"). This is usually during the university years, MSc and PhD studies, when the research interests are formed and shaped. Very often, this happens under the influence of professors, supervisors, older friends, and books. That time is of paramount importance for a young person, since the foundations of the future career steps, skills, and knowledge are implicitly created. As a rule, that period is the time of really hard work in the laboratories and libraries, search for various good books and articles to learn new things, accept and understand new concepts, "digest" them, and use them in the future research.

Also, in the life of every scientist, there is a time when he looks back upon his younger (or better—in a way) years. Then the understanding comes that some things were not done in the best way. For example, some books could have been missed for some reasons, or the time was not organized efficiently. And then the thought is coming to help young researchers make their scientific path smoother. When both authors were going through their PhD studies—chronologically and geographically it was in different times and countries—they felt a huge gap between the university courses on atomic physics and quantum mechanics and specialized books on atomic spectroscopy, theory of crystal field, and group theory. Many different books had to be consulted at that time to make a (more or less) clear picture of why different crystals and different impurity ions behave in remarkably different ways, to understand their main spectroscopic properties, to describe and quantify them and, finally, to start real research on the basis of that acquired knowledge. Going through many books on the same subject has a clear and enriching advantage of looking at the same topic from the perspectives of different authors. The price to be paid for that—especially if we speak about quantum mechanics and spectroscopy—is fighting with different conventions, notations, systems of units, numerical factors, normalizations, etc.

In an attempt to fill in this gap between the university courses on physics and research on the optical properties of the transition metal and lanthanide ions, we wrote this book on theoretical spectroscopy of these ions in a free state and in crystals. We hope that having such a single book with description of the energy levels' formation (in a free state), their splitting (in crystal fields), group theory in its application to spectroscopy, and examples of the application of all that to real optical materials would help young researchers to understand these topics clearly. We tried to write the book in as simple way as possible (although, of course, a certain level of quantum mechanics and calculus knowledge would be required to feel comfortable when reading the book). The book contains many examples of the application of those theoretical concepts to the real physical systems and those examples are based on the original authors' publications. It is hoped that the book will be a bridge to more advanced quantum-mechanical books, many of those are cited here or mentioned as a literature for further reading.

We also believe that the book will be helpful to the experimental scientists to refresh (or to get familiar with) basic theoretical concepts that may be useful for a proper interpretation of the experimental spectroscopic results.

Writing this book was an awesome adventure of going back in time to our PhD years—trying to recollect what the most difficult topics were for us and at the same time contacting our current students to understand what the most difficult topics are for them. The content of the book is based on the lectures on spectroscopy of the transition metal and rare earth ions, which the authors have given (and continue to give) at the University of Tartu in Estonia and Chongqing University of Posts and Telecommunications in China. Besides, as a guest professor, one of the authors (MGB) taught a number of relevant topics at Kyoto University in Japan, Lanzhou University and South China University of Technology in China, and Jan Długosz University in Częstochowa, Poland.

We also would like to express our sincere gratitude to all our numerous colleagues and friends worldwide. We simply cannot mention their names here because of the lack of space on the book pages—but we truly remember all of them! Fruitful and stimulating discussions with them on a variety of topics—science, teaching, culture, art, sport, history, literature, food, etc.—were extremely

interesting and enjoyable! Science is an amazing thing: In addition to real pleasure of being involved into solving interesting scientific problems, it gives a person a unique chance to travel a lot, to be exposed to different cultures, to see exciting places all over the globe, and to appreciate breathtaking rare beauty of our world—this must be cherished!

Being unable to name here all our friends and colleagues, we wish, however, to mention our first teachers—they introduced us to the field of spectroscopy of the transition metal and rare earth ions and they made us in the way we are now.

MGB gratefully acknowledges very important influence of Dr. V. V. Zhorin and late Professors A. G. Avanesov, V. A. Lebedev, and V. F. Pisarenko from his *alma mater* (Kuban State University, Krasnodar, Russia). He is also much indebted to his mother and his late father, who was a school physics teacher. Many thanks are due to Professor N. M. Avram (West University of Timisoara, Romania) for long friendship and first international visit to his place, back in September of 2000.

CGM gratefully acknowledges the help on his earlier scientific career offered by Professors S.-D. Xia, M. Yin, C.-K. Duan (University of Science and Technology of China, Hefei, China), P. A. Tanner (City University of Hong Kong, Hong Kong, China), and M. F. Reid (University of Canterbury, Christchurch, New Zealand).

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At last, but by no means at least, we would like to thank sincerely our families—for their everlasting patience, support, and understanding during our whole scientific careers! We owe them a lot, if not everything!

And—with all that said—*lectori benevolo salutem!*

**Mikhail G. Brik**

**Chong-Geng Ma**

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