



Computational Quantum Chemistry II - The Group Theory Calculator: 2

Charles M. Quinn, Patrick Fowler, David Redmond

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Modern Computational Quantum Chemistry is indispensable for research in the chemical sciences.

Computational Quantum Chemistry II - The Group Theory Calculator describes the group theory that the authors have developed in the past twenty-five years and illustrates how this approach, known as the 'Spherical Shell' method, can be applied to solve a variety of problems that benefit from a group theory analysis.

To complement the theory, the book is supplied with a CD-ROM (Windows™ application), on which interactive files, based on EXCEL spreadsheet technology controlled by Visual Basic code, can be used to perform straightforwardly group-theory analyses for direct application to the simplification of physical problems in Chemistry, Physics and even Engineering Science.

The **Group Theory Calculator Web page** is located at http://www.chemistry.nuim.ie/gt_calculator.htm.

The primary purpose of this Web page is to identify and resolve any problems encountered while using the MS EXCEL files on the CD-ROM (included with the book). The Web page is maintained by Charles M. Quinn and allows readers to gain updates and news relating to this publication.

- * A comprehensive description of the authors' revolutionary group theory and structural chemistry methodology
- * A unique reference/ teaching work together with a CD-ROM filled with powerful interactive files that can be applied to solve group theory problems
- * Valuable companion for instructors, designers and students
- * Contains powerful calculators that are simple to use and do not require detailed knowledge for their application



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