Scientific Research Publishing

Open Journal of Physical Chemistry, 2026, 16(4), 77-80
https://www.scirp.org/journal/ojpc
ISSN Online: 2162-1977
ISSN Print: 2162-1969

Book Review of *Mathematical Methods for Molecular Science*: *Theory and Applications, Visualizations and Narrative* (Japanese Edition)

Takashiro Akitsu

Department of Chemistry, Faculty of Science, Tokyo University of Science, Tokyo, Japan
Email: akitsu2@rs.tus.ac.jp

How to cite this paper: Akitsu, T. (2026) Book Review of *Mathematical Methods for Molecular Science: Theory and Applications, Visualizations and Narrative* (Japanese Edition). *Open Journal of Physical Chemistry*, **16**, 77-80.
https://doi.org/10.4236/ojpc.2026.164006

Received: October 14, 2026
Accepted: November 7, 2026
Published: November 10, 2026

Copyright © 2026 by author(s) and Scientific Research Publishing Inc.
This work is licensed under the Creative Commons Attribution International License (CC BY 4.0).
http://creativecommons.org/licenses/by/4.0/

Open Access

Abstract

This paper presents a book review of the Japanese edition of *Mathematical Methods for Molecular Science* by John E. Straub, translated by Tetsuro Nagai and co-workers. Recent changes in Japan's high school mathematics curriculum have created a gap for chemistry students entering university, particularly regarding linear algebra. This textbook effectively addresses this challenge by integrating foundational mathematics such as calculus, differential equations, Fourier transforms, and linear algebra into a unified framework centered on molecular science. Highly relevant to fields like crystallography and coordination chemistry, the book utilizes practical chemical examples and intuitive visual representations instead of abstract theory. It serves as an invaluable resource for undergraduate students, educators, and researchers seeking to bridge the boundaries between mathematics and contemporary molecular science.

Keywords

Mathematical Chemistry, Mathematics Education, Matrix Algebra, Group Theory and Symmetry, Japanese Translation

1. Book Review

Recent changes in mathematics education in Japan have significantly influenced the preparation of students entering university chemistry programs. Topics such as matrices and linear transformations, which were previously included in high school curricula, are no longer taught in the same way, while greater emphasis has been placed on statistics and the complex plane. At the same time, the growing importance of data science has increased the need for mathematical literacy

among students in the natural sciences. Under these circumstances [1], many students encounter a gap between introductory university mathematics courses and the mathematical tools required in chemistry and related disciplines.

The Japanese translation of *Mathematical Methods for Molecular Science* by John E. Straub [2], translated by Tetsuro Nagai and co-workers and published by Kagaku-Dojin, provides a timely introduction to mathematical concepts from the perspective of molecular science. The book is intended for students and researchers who wish to understand not only the mathematical foundations (high school or university freshman level) of chemical phenomena but also the practical applications of mathematical methods in modern molecular science. For example, Chapter 14 of the Japanese edition is translated as "Matrices and Matrix Algebra" rather than "Matrices and Linear Algebra", employing more natural, less abstract terminology in Japanese language.

The book consists of sixteen chapters that cover a broad range of topics, including calculus, differential equations, linear algebra, probability, statistics, and symmetry. Rather than treating these subjects independently, the author presents them within a common framework centered on molecular science. Throughout the text, mathematical concepts are illustrated with examples drawn from chemistry, physics, and materials science, making the content accessible to readers with scientific interests. Interestingly, Figure 1.8 indicates a $\ln[p(T)]$ vs $1/T$ 'straight' line on a semi-logarithmic plot, which is frequently used in chemical experiments.

From the perspective of crystallography, Chapter 13, which deals with Fourier series, Fourier transforms, and harmonic analysis, is particularly noteworthy. Fourier transforms as well as phase problem form the theoretical basis for determining electron density distributions from diffraction data, yet many students encounter these methods only through software packages and automated procedures [3]. The chapter provides a clear explanation of the underlying mathematical principles and their physical significance, helping readers understand how diffraction experiments are connected to structural models.

The final chapters, covering matrices, eigenvalues, geometric transformations, and molecular symmetry are especially relevant to students of inorganic and coordination chemistry [4]. Symmetry operations, point groups, and group theory are fundamental concepts in these fields, but they are often introduced after only limited exposure to matrix methods. For students who have not previously studied matrices in depth, the relationship between matrix operations and molecular symmetry may appear abstract.

This book addresses that difficulty by introducing matrices in a practical context and demonstrating how they can be used to describe rotations, reflections, and other geometric transformations. The discussion of eigenvalues and diagonalization further supports the understanding of symmetry-based approaches used in spectroscopy, crystallography, and quantum chemistry [5]. Readers are able to see how mathematical concepts are applied in the analysis of molecular structures and properties.

Another strength of the book is its extensive use of visual representations and worked examples. Abstract mathematical ideas are frequently accompanied by graphical illustrations, making it easier for readers to connect equations with physical and chemical phenomena. This approach is particularly valuable for students whose primary interests lie in chemistry rather than mathematics.

The publication of the Japanese edition is likely to be welcomed by students and educators alike. As interdisciplinary research continues to expand, the ability to communicate across the boundaries of mathematics, chemistry, physics, and data science has become increasingly important. In this context, *Mathematical Methods for Molecular Science* provides a useful resource for understanding how mathematical methods contribute to contemporary molecular science.

Overall, this book offers a well-organized introduction to the mathematical foundations of molecular science. It will be valuable not only for undergraduate and graduate students in chemistry and related disciplines but also for researchers seeking a broader understanding of the mathematical tools commonly used in modern scientific research.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

[1] Akitsu, T. (2016) High School Science Selection and Literacy of University Chemistry. *Kagaku to Kyoiku*, **64**, 588-591. (In Japanese)

[2] Straub, J.E. (2026) Mathematical Methods for Molecular Science. Kagaku-Dojin Publishing. 360 pp. Japanese Translation Edition. Translated by Nagai, T., Yoshida, K. and Fujisaki, H.

[3] Hammond, C. (2015) The Basics of Crystallography and Diffraction (International Union of Crystallography Texts on Crystallography, No. 21). 4th Edition, Oxford University Press.

[4] Borchardt-Ott, W. (2011) Crystallography: An Introduction. 3rd Edition, Springer. Translated by Gould, R. O.

[5] Yang, S.-K. (2026) Gyoretsu to henkan-gun [Matrices and Transformation Groups] (Key Points of Mathematics for Science and Engineering, Vol. 8). Iwanami Shoten. (In Japanese)

Appendix: The Cover of *Mathematical Methods for Molecular Science*: *Theory and Applications, Visualizations and Narrative* (Japanese Edition)

