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Group Theory with Mathcad

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Mathcad (*1*) is a comprehensive, inexpensive program for doing numeric and symbolic mathematics. Available for both Windows and Mac OS, Mathcad has an appealing, user-friendly, graphical interface. It has a wide variety of applications in the undergraduate chemistry curriculum, but is especially useful in the mathematically intensive courses traditionally found in the physical chemistry sequence (*2–5*). Previous publications by the author presented applications of Mathcad in the area of quantum mechanics (*6–8*). The collection of documents presented here use Mathcad to solve problems in group theory.

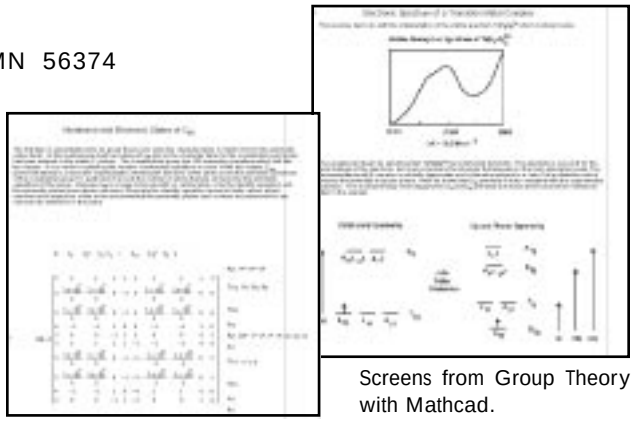
Mathcad has a powerful array of matrix manipulation commands that make it an ideal programming environment for applying mathematical group theory to chemistry problems. To illustrate this capability, Mathcad is used to do symmetry analyses on a number of examples involving vibrational and electronic spectroscopy and chemical bonding.

The examples treated in this series deal only with molecules that belong to the finite point groups. Most examples deal with molecules having moderate to high symmetry—C_{2v} to I_h. Obviously all finite groups are not considered, but the most frequently encountered symmetries receive sufficient attention. Fortunately Mathcad worksheets are easy to prepare and edit, so the worksheets included in this series can serve as templates for a large number of additional exercises. Once a worksheet has been created for a particular point group, it can be used for any molecule with that symmetry with minor modification.

Among the exercises included are:

- Analysis of the Vibrational and Electronic States of C_{60}
- Cubane, Tetrahedrane, and XeF_4: Molecular Structure from Vibrational Spectroscopy
- Analysis of the Electronic Spectrum of a Transition Metal Complex
- Hybridization of Atomic Orbitals with Group Theory
- Miscellaneous Exercises

For each of the major areas listed above, a number of additional exercises are recommended that require some editing of the template Mathcad worksheet.



Screens from Group Theory with Mathcad.

References

Harris, D. C.; Bertolucci, M. D. *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*; Dover : New York, 1989.

Cotton, F. A. *Chemical Applications of Group Theory*, 3rd ed.; Wiley Interscience: New York, 1990.

Literature Cited

1. Mathcad; MathSoft, Inc., 101 Main Street, Cambridge, MA 02142; telephone: 1-800-628-4223.
2. Coleman, W. F. *J. Chem. Educ*. 1990, *67*, A203.
3. Adravkoski, Z. *J. Chem. Educ.* 1991, *68*, A95.
4. Rioux, F. *J. Chem. Educ.* 1992, *69*, A240.
5. Turner, O. E. *J. Chem. Educ.* 1993, *70*, A185.
6. Rioux, F. *J. Chem. Educ. Software*, 1993, *1D*, No. 2.
7. Rioux, F. *J. Chem. Educ. Software*, 1995, *3D*, No. 2.
8. Rioux, F. *J. Chem. Educ. Software*, 1997, *9C*, No. 1.

How To Use Group Theory with Mathcad

Group Theory with Mathcad is intended for use by students in inorganic and physical chemistry. It could be used in class to present problems, or be used individually by students, perhaps as part of a homework or laboratory exercise.

Hardware and Software Requirements

Mathcad is required and is not included in this issue. Versions of the software for both Mac OS and Windows are included. Hardware and software requirements for Group Theory with Mathcad are listed in Table 1.

Table 1. Hardware and Software Required for Group Theory with Mathcad

Computer	CPU	RAM	Drives	Free Disk Space	Graphics	Operating System	Other Software
Mac OS Compatible	68030 or higher with FPU or Power Mac	≥ 16 MB	Hard Drive, High-density (1.44MB) floppy drive	1 MB*	≥ 256 colors, 640 × 480	System 7 or higher	Mathcad 6 or Mathcad PLUS 6 for Mac OS
Windows Compatible	80386 or higher, Math coprocessor recommended	≥ 8 MB	Hard Drive, High-density (1.44MB) floppy drive	1 MB*	≥ 256 colors, 640 × 480	Windows 3.1 or Windows 95	Mathcad version 4 or later