JCE Software

edited by
Jon L. Holmes
Nancy S. Gettys
University of Wisconsin–Madison
Madison, WI 53706

Advanced Chemistry Collection, 2nd Edition

Abstract of Special Issue 28, 2nd Edition, a CD-ROM (for Students)

Are you teaching courses beyond the general-chemistry level? Would you like your students to take advantage of software designed and peer-reviewed by teachers such as you? If so, consider adopting the *JCE Software* Advanced Chemistry Collection (ACC). This CD-ROM for Mac OS and Windows contains software that will enhance student learning in analytical, inorganic, organic, and physical chemistry courses, biochemistry courses, and many others. ACC includes both previously published and new peer-reviewed software on a single CD-ROM for convenient access by students. The programs included and the broad range of topics they address are listed in Table 1. The abstract for Spec UV–Vis, a new program not previously published by *JCE Software* is found on page 1560. Abstracts for other programs are available from the *JCE Software* Web site (*http://jchemed.chem.wisc.edu/JCESoft/Programs/ACC/contents.html*).

ACC is modeled on the General Chemistry Collection (*1*), now in its 5th edition. We expect students will find the programs included in ACC useful tools for learning chemistry outside the classroom as they progress through the chemistry curriculum.

New Features in This Edition

Advanced Chemistry Collection, 2nd edition includes all of the contents of the first edition (*2*), with the additions and updates listed below. The entire contents appear in Table 1.

- Spec UV–Vis: An Ultraviolet–Visible Spectrophotometer Simulation—a new program for Windows
- Inorganic Molecules: A Visual Database for Mac OS
- Updated versions of two programs for Windows: DYNAM and Equilibrium Calculator

Licensing, Volume Discounts for Adoptions

ACC is intended for use by individual students. Institutions and faculty members may adopt ACC 2nd edition as they would a textbook. We can arrange for CDs to be custom packaged with laboratory manuals or other course materials or to be sold to students through the campus bookstore. The cost per CD can be quite low when large numbers are ordered (as little as $3 each), making this a cost-effective method of providing students access to the software they need whenever and wherever they desire. Network licenses to distribute the software to your students via your local campus network can also be arranged. Contact us for details on purchasing multiple-user licenses.

Table 1. Contents of the Advanced Chemistry Collection

Software for Mac OS and Windows	Topics
Alkanes in Motion	Molecular models, Molecular motion, Molecular vibration
Enriching Quantum Chemistry with Mathcad	Quantum chemistry, Mathcad
Group Theory with Mathcad	Group theory, Mathcad
Schroedinger.m	Quantum chemistry, Mathematica
Solid State Structures	Solid state, Structural chemistry
Software for Mac OS	**Topics**
Acid–Base Package	Titration curves, Buffers, Alpha plots
Coordination Compounds	Octahedral complexes, Structural isomers, Inorganic nomenclature
Frost Diagrams: A Tool for Predicting Redox Reactions	Oxidation-reduction, Frost diagrams
*Inorganic Molecules: A Visual Database	Molecular models, Molecular orbitals, VSEPR theory
MacMS: A Mass Spectrometer Simulator	Mass spectrometry
Molecular Dynamics of the F+H_2 Reaction	Reaction dynamics
MolVib 2.0	Molecular vibrations, Normal modes
Organic Nomenclature	Organic nomenclature
Pericyclic Reactions: FMO Approach	Pericyclic Reactions, Molecular orbitals
Precision of Calculated Values	Experimental error
Proton NMR Spectrum Simulator	NMR
PTRJ	Kinetics, Theoretical chemistry
Reaction Dynamics	Reaction dynamics
Symmetry Elements and Operations	Symmetry
Viscosity of Polymer Solutions	Density, Polymers
Software for Windows	**Topics**
Buffers Plus	Alpha plots, Buffers, Titration curves
†DYNAM: Molecular Dynamics Simulator	Molecular motion
Enzyme Lab	Enzymes, Reaction rate
†Equilibrium Calculator	Equilibrium calculations
G and S	ΔH, ΔS, ΔG calculations, Entropy
GC Instrument Simulator	Gas chromatography
HIPPO-CNMRS	NMR
HPLC for Windows	Chromatography
Simulation of the Physical Chemistry of Gas Chromatography	Gas chromatography
SPECPNMR	NMR
*Spec UV–Vis: An Ultraviolet-Visible Spectrophotometer Simulation	Ultraviolet–Visible spectroscopy
TorAD for HyperChem/Excel	Molecular motion, Rotation about torsional angle
Viscosity Measurement	Density, Viscosity
WinDNMR: Dynamic NMR Spectra	NMR
Window on the Solid State: Parts I–IV	Solid state
Winspec: Microwave Spectroscopy Tutor	Microwave/rotational spectroscopy

*New additions. †Updates from previous edition.

Table 2. General hardware and software requirements for the Advanced Chemistry Collection.

Computer	CPU	RAM	Drives	Graphics	Operating System	Other Software (required by one or more program)
Mac OS Compatible	Power Mac	≥ 32 MB	CD-ROM; Hard Drive	≥ 256 colors; ≥ 800 × 600	System 7.6.1 or higher	Acrobat Reader (included); Mathcad; Mathematica; MacMolecule2; QuickTime 4; HyperCard Player
Windows Compatible	Pentium	≥ 32 MB	CD-ROM; Hard Drive	VGA; SVGA with ≥ 256 colors; ≥ 800 × 600	Windows 98, 95, 2000, NT 4	Acrobat Reader (included); Mathcad; Mathematica; PCMolecule2; QuickTime 4; HyperChem; Excel

Price and Ordering

An order form inserted in this issue provides prices and other ordering information. For orders of 20 or more CDs, contact *JCE Software* for bulk order prices.

For more information, contact *JCE Software*, email: *jcesoft@chem.wisc.edu*. Information about all of our publications (including abstracts, descriptions, updates, etc.) is available from our World Wide Web site at

http://jchemed.chem.wisc.edu/JCESoft/

Acknowledgment

ACC contains the work of many authors. The time and effort of these dedicated chemistry educators in producing these programs is gratefully acknowledged by the editors, along with the authors' generosity in contributing their work to the chemistry education community by submission to *JCE Software*. Thanks are also due the many peer reviewers who volunteered their time to test these programs, and the thousands of chemistry instructors all over the world who have made these programs available to their students. Their input has been invaluable in program development, revisions, and updates.

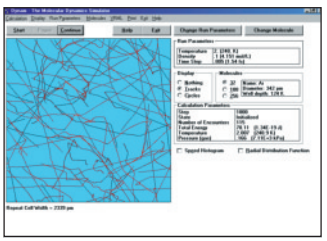
Hardware and Software Requirements

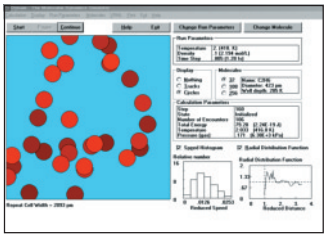
System requirements are given in Table 2. Some programs have additional special requirements. Please see the individual program abstracts at *JCE Online* or the documentation included on the CD-ROM for more specific information.

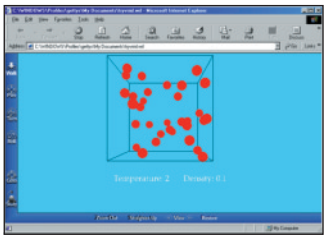
Literature Cited

1. General Chemistry Collection, 5th ed.; *J. Chem. Educ. Software*, **2001**, *SP16*.
2. Advanced Chemistry Collection; *J. Chem. Educ. Software*, **2001**, *SP28*.

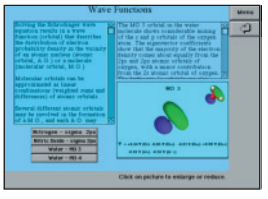
Selected Images from Advanced Chemistry Collection

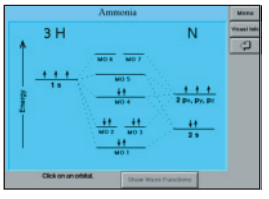






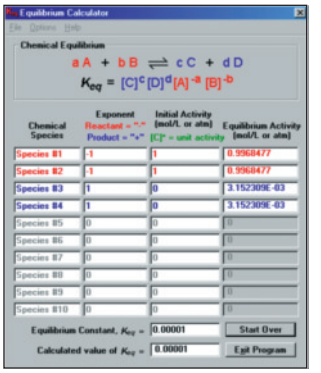
DYNAM shows the ways that the motion of atoms or molecules can be displayed (from left to right): with the path traced, as a 2-dimensional animation, and as a 3-dimensional VRML animation. The VRML animation is a new feature in the update.





Inorganic Molecules: A Visual Database provides information about molecular orbitals and wave functions for advanced students.

The update of Equilibrium Calculator allows more flexibility in the number of reactants and products.



Spec UV–Vis: An Ultraviolet–Visible Spectrophotometer Simulation

Nikos Papadopoulos*, Maria Limniou, Giannis Koklamanis, Apostolos Tsarouxas, and Mpampis Roilidis

Laboratory of Physical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, 54006 Thessaloniki, Greece; **npapado@chem.auth.gr*

Stephen W. Bigger

School of Life Sciences and Technology, Victoria University of Technology, Melbourne, 8001, Australia

SpecUV–Vis is a Windows compatible computer program that simulates an ultraviolet (UV)–visible spectrophotometer (*1–4*) with a wavelength range of 350 to 750 nm. The program has two operational modules.

The Single-Beam Spectrophotometer (SBS) Module (see Fig. 1) enables the user to make separate absorbance or transmittance measurements at 1-nm intervals within the wavelength range of the simulated instrument. The procedure for operating the SBS Module mimics that required for most single-beam instruments. The user must switch on the light source, select the wavelength, set the transmittance zero reading, use a reference to set the absorbance zero reading, prepare a sample, and place it in the instrument to make a reading, not forgetting to close the cover of the cell compartment before taking the reading.

The Double-Beam Spectrophotometer (DBS) Module (see Fig. 2) enables the user to scan through the entire wavelength range of the instrument and produces either an absorbance or transmission spectrum of the selected sample. Data are recorded at 1-nm intervals and the displayed spectrum can be saved as an ASCII data file for import into a suitable graphics program such as Microsoft Excel. Both modules incorporate a Sample Preparation Area (SPA) that contains five acid–base indicators: thymol blue, methyl orange, bromophenol blue, bromothymol blue, and phenol red. The concentration and pH of a selected indicator can be varied and the software reproduces accurately the color of the indicator under the set conditions.

The instruction manual that accompanies the software includes:

- detailed notes for using the simulator
- background information on UV–visible spectrophotometry and instrumentation
- suggested exercises for each module
- notes for instructors that relate to the exercises

The software and its accompanying manual can be used to illustrate the recording of an absorption spectrum and the Beer–Lambert law (*5–7*) as well as various aspects of acid–base indicators such as the spectrophotometric determination of pK_a (*8*), the isosbestic point (*6, 9*), and distribution diagrams (*10, 11*).

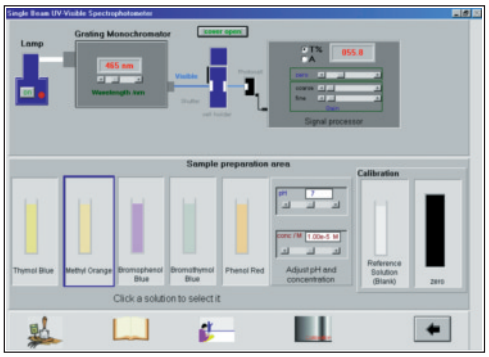


Figure 1. The Single-Beam Spectrophotometer (SBS) Module

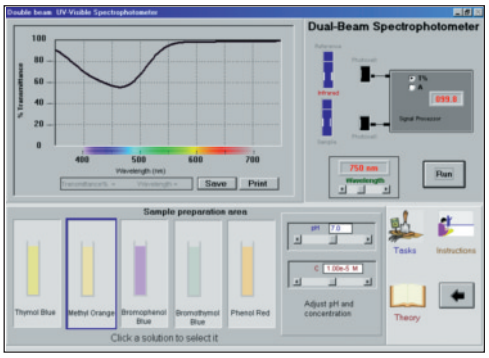


Figure 2. The Double-Beam Spectrophotometer (DBS) Module

Literature Cited

1. Shiowatana, J. *J. Chem. Educ.* **1997**, *74*, 730.
2. Altemose, I. R. *J. Chem. Educ.* **1986**, *63*, A216, A262.
3. Piepmeier, E. H. *J. Chem. Educ.* **1973**, *50*, 640.
4. Lott, P. F. *J. Chem. Educ.* **1968**, *45*, A89, A169, A182, A273.
5. Skoog, D. A.; West, D. M.; Holler, F. J. *Fundamentals of Analytical Chemistry*, 7th ed.; Saunders College Publishing: Fort Worth, TX, 1996, Chapters 22–24.
6. Christian, G. D. *Analytical Chemistry*, 5th ed.; Wiley: New York, 1994; Chapter 14.
7. Kennedy, J. H. *Analytical Chemistry–Principles*, 2nd ed.; Saunders College Publishing: New York, 1990; Chapters 11, 12.
8. Patterson, G. S. *J. Chem. Educ.* **1999**, *76*, 395.
9. Harris, D. C. *Quantitative Chemical Analysis*, 5th ed.; Freeman: New York, 1997; Chapters 19, 20.
10. Butler, J. N. *Ionic Equilibrium—A Mathematical Approach*; Addison-Wesley: Reading, MA, 1964; Chapter 5.
11. Sawyer, C. A.; McCarty, P. L.; Parkin, G. F. *Chemistry for Environmental Engineering*, 4th ed.; McGraw-Hill: Singapore, 1994; Chapter 4.