

Computational Chemistry for Chemistry Educators



EDU 102

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Two Approaches

1. Computational (Chemistry Education)

- Use of technology to teach chemical concepts
- More: -Visual -Interactive -Interesting(?)

→ If “*a picture is worth a thousand words*”,
then.... “*a well-done java applet is worth a
thousand pictures*”

2. (Computational Chemistry) Education

- Molecular modeling
- Kinetics using MathCad, Excel, or Vensim PLE
- Teaching a *tool* to learn some Chemistry

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Computational (Chemistry Education)

- Teach the same subjects in a different way
 - Improved visualization
 - Experimentation enabled (What if.....? questions)
- Get students involved in an *interactive* manner
- Lecture / Lab / Recitation / Homework

• Resources: CSERD

Computational Science Education Reference Desk

- A Pathways project (DUE 0435187) of NSF’s National Science Digital Library

– <http://www.shodor.org/refdesk/>

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CSERD

- CSERD attempts to:
 1. Provide a **collection** of quality resources from the Internet
 2. Provide a forum for the **review** of catalog items by both users and expert reviewers
 - Users are encouraged to review sites they use
 3. **Create** original computational science resources for use in education
 - Users can submit items for inclusion in the collection

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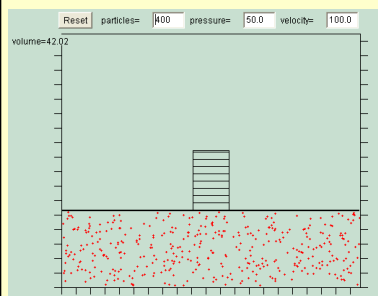
Searching CSERD

- Can browse the catalog by:
 - Subject (Chemistry, Physics, etc.)
 - Keyword (Spectroscopy, Ideal Gas law, etc.)
 - Audience (Student, Educator, etc.)
 - Education level (K-16)
 - Resource Type (Software, text, applet, etc.)
- Over 220 Chemistry sites in the database
 - Users are encouraged to add useful sites
 - New materials can be added
 - Applets, lesson plans based on a site, etc.

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Examples of CSERD Contents

- Molecular Model for an Ideal Gas



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Studies:
 $V \propto T$
 $V \propto n$
 $V \propto P^{-1}$
Conclude:
 $PV \propto nT$ or
 $PV = nRT$

Examples of CSERD Contents

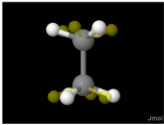
- **Symmetry Tutorial**
 - Symmetry Operations
 - Introduction
 - Identity
 - Reflection
 - Inversion
 - Proper Rotation
 - Improper Rotation
 - Example Molecules
 - Water
 - Benzene
 - Ethane (staggered)
 - Methane
 - Information
 - About this Tutorial
 - Technical Details
 - References and Links

Symmetry Tutorial - Improper Rotation

Improper Rotation (S_n)

An improper rotation is performed by rotating the molecule $360^\circ/n$ followed by reflection through the plane perpendicular to the rotation axis. If the resulting configuration is indistinguishable from the original, we say there exists an n -fold improper rotation axis (or S_n axis) in the molecule. Some example molecules are shown below.

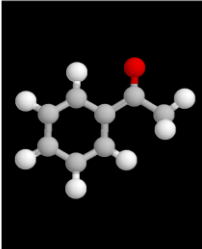
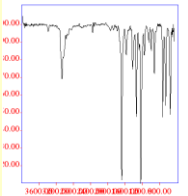
Staggered Ethane (C_2H_6) -- S_6 axis



Elements show improper rotation axis (S_6)
 show plane perpendicular to S_6
Operations

This project supported by NSF-DUE-0053070

Examples of CSERD Contents

- **Infrared Spectroscopy – Web-Based**
 - IDENTIFYING SPECTRAL MODES**
by Eric Motyka, Paul M. Lahti, and Robert Lancashire
Copyright © 1999 by Paul Lahti and Robert J. Lancashire -- commercial use prohibited without written permission.
 - Acetophenone IR Spectrum and Vibrations
Macintosh? Spin Spacefill Balls & Sticks Sticks
 - INFRARED SPECTRUM: Acetophenone 0.7574
EPA IR VAPOR PHASE LIBRARY: 1.44131
 - TRANSMITTANCE
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CSERD Reviews

- **Reviewer:** Account creation/login required
 - Performs reviews of catalog items
 - **Structured** and **freeform** reviews possible
 - Structured:
 - Three types: Verification, Validation, and Accreditation (VV & A)
 - Online guide to review types provided
 - In-depth look at the usability of the item
 - Free-form:
 - Paragraph form
 - Usually provides an opinion about a site

(Computational Chemistry) Education

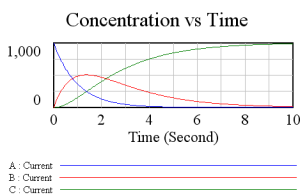
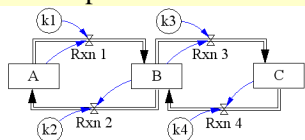
- Teach a modeling tool to explore chemistry
 - Example 1: Chemical Kinetics
 - Tools: Spreadsheet, Mathcad, Vensim PLE
- Vensim PLE: <http://www.vensim.com/venple.html>
- **Free** system dynamics software package for personal and educational use
 - Used in addition to kinetics experiments, allows more broad investigation of the field
 - Can handle simple to complex rate laws
 - Graphical user interface reduces math dependence

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Vensim PLE

- Example: $A \leftrightarrow B \leftrightarrow C$



1st order
Reversible 1st Order
Consecutive 1st Order
-Disequilibrium
-Transient equilibrium
-Secular equilibrium
Reversible
Consecutive 1st Order

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(Computational Chemistry) Education

- Example 2: Molecular modeling
 - Tools: Many available, some are free
 - Nice, free combination: WebMO/GAMESS
 - Graphical interface: WebMO (Pro version = \$1000)
 - Computational engine: GAMESS

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CCCE Labs

Computational Chemistry for
Chemistry Educators
A Program of the National Computational Science Institute


Location: [CCCE Home](#) > [Labs](#)

Name of the Session	CAChe	Spartan	Chem3D	Hyperchem	PC Model	GaussView/ Gaussian	WebMO	Spreadsheet
1. Introduction To Computational Chemistry	Link	Link	Link	Link	Link	Link	Link	
2. Basis Sets								Link
3. Choice of Theoretical Method	Link	Link	Link	Link	Link	Link	Link	
4. Single Point Energies	Link	Link	Link	Link	Link	Link	Link	
5. Electron Densities and Electrostatic Potentials	Link	Link	Link	Link	Link	Link	Link	
6. Modeling in Solution	Link	Link	Link	Link	Link	Link	Link	
7. Computing Spectroscopic and Thermochemical Properties	Link	Link	Link	Link	Link	Link	Link	
8. QSAR / QSPR	Link	Link	Link	Link	Link	Link	Link	Link
9. Transition States	Link	Link	Link	Link	Link	Link	Link	
11. Biochemical Applications of Computational Chemistry	Link							
10. Computational Study of System Dynamics				Spreadsheet	STELLA	Berkeley-Madonna	Vensim	PLE MathCad

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