

EDU 110 lab

Journal of Chemical Education



Project SERAPHIM

Project SERAPHIM began over 25 years ago as a clearinghouse for software and materials for computational chemistry. Membership fees supported the software clearing house, teacher workshops, and summer fellowships for software development. Software was distributed at a modest cost to members. A catalog listing several hundred different programs written for Apple II, Macintosh, and MS/PC-DOS is available at the <http://ice.chem.wisc.edu/seraphim> website. These programs include:

- data bases–nmr library and experiments published in *JCE*
- data analysis tools–significant figures, least squares analysis, dimensional analysis, spreadsheet calculations, and integration techniques
- chemical clip art
- teaching support–quiz preparation and computer testing
- simulation problems–wastewater treatment and water pollution
- tutorials and games
- laboratory–experiment simulations, analytical techniques, and instrument interfacing
- core curriculum topics–states of matter (gases and crystals), nomenclature and formulas, stoichiometry (chemical equations, titrations, limiting reactants, and equilibria), thermochemistry, atomic structure (electron configurations, orbitals, and SCF calculations), chemical bonding (molecular orbitals, HF calculations, Hückel calculations, and group theory), spectroscopy (atomic, nmr, and esr), dynamics (distribution of gas molecular speeds and chemical reaction kinetics), and descriptive chemistry (acid-base, redox and electrochemistry, complexes, qualitative analysis, reaction prediction, organic molecules, biochemistry, polymers, and industrial chemistry)

Currently, all Project SERAPHIM materials are available as free downloads from the website.

JCE Software

The *JCE Software* resulted from a collaboration between *JCE* and Project SERAPHIM with initial support from the Dreyfus Foundation. For over 20 years the motto of the journal has been “*JCE Software* is not *about* software, *it is* software”. Originally, the journal was published as three series for Apple II, Macintosh, and MS/PC-DOS users and later a fourth series was added for Windows users. The software and corresponding printed materials were sent to subscribers twice a year. Currently, in addition to various video materials, *JCE Software* offers over 15 “special issue” software collections covering laboratory and supplementary classroom materials for Macintosh and Windows users:

- general and advanced chemistry collections–student-designed collections featuring animations, simulations, and computational tools for acid-base chemistry, equilibria, spectroscopy, crystal structure, and quantum mechanics
- *Chemistry Comes Alive!* collections–movies, pictures, and animations of reaction types, stoichiometry, states of matter, thermodynamics and electrochemistry, organic and biochemistry, and laboratory techniques
- collections on specific topics–periodic table, laboratory techniques, nmr, solid state surfaces, material science, crystallography, and problem-based learning

Many of the software programs are web-ready and appropriate licensing is available for local intranets. Much of the older software for MS/PC-DOS is available as free downloads at <http://JChemEd.chem.wisc.edu> for *JCE* subscribers.

Sample Content from the General Chemistry Collection Special Issue 16

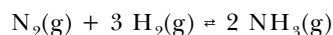
Alkanes in Motion

Spec UV_Vis

Orbitals

Equilibrium Calculator

Consider the important reaction (Haber process)



for which $K_p = 1.64 \times 10^{-4}$ at 400 °C. Starting with 2.5 bar N_2 and 7.5 bar H_2 , what is $P(\text{NH}_3)$ at equilibrium?

Usual solution (using ICE table):

	N_2	+	3H_2	\rightleftharpoons	2NH_3
initial	2.5		7.5		0
change	-x		-3x		+2x
equilibrium	$2.5 - x$		$7.5 - 3x$		2x

$$K = \frac{P(\text{NH}_3)^2}{P(\text{N}_2) P(\text{H}_2)^3} = \frac{(2x)^2}{(2.5 - x)(7.5 - 3x)^3} = 1.64 \times 10^{-4}$$

Who wants to solve a quartic equation for x? Phooey!

Entries in Equilibrium Calculator

1st row: N_2 , -1, 2.5 (should be red)

2nd row: H_2 , -3, 7.5 (should be red)

3rd row: NH_3 , 2, 0 (should be blue)

Equilibrium Constant: 1.64E-4

Click "Calculate Now" and get answer for equilibrium pressures of 2.32, 6.96 and 0.358 bar and a calculated value of K of 0.000164 as a check.

Obviously we still want to teach equilibrium calculations, but for hard ones—here is something that makes the math easy.

Buffers Plus

Click option "F Plot acid-base titration curves"

from the menu choose "pKa Table"

choose acetic acid and click "Select"

titration curve appears

repeat using phosphoric acid

Great for quick calculations of acid/base/buffer quantities. Titration curves easily replace the static curves in textbooks and can be used as a quick teaching tool.

Logon to JCE websites