Innovations in the Teaching of Analytical Chemistry: How they have evolved

Gary D. Christian
Department of Chemistry
University of Washington
Seattle, WA 98195-1700 USA
christian@chem.washington.edu

Workshop on the Contents and Perspectives of Analytical Chemistry in Spanish Universities

Alcalá de Henares, Spain, April 10, 2014

Sponsored by the Spanish Society for Analytical Chemistry

1. The importance of analytical chemistry
2. How it developed
3. The tools we use
4. The evolution of textbooks
5. What is taught and how it has changed
6. Some (new) ways we teach (How do we teach it?)
7. Teaching social responsibility in AC
8. Teaching resources in the analytical sciences

Why do we need analytical chemists?

- Everything is made of chemicals

- We need to find information about them

- Analytical chemists do this for us

Charles N. Reilley

“Analytical chemistry is
what analytical chemists do”

(See R.W. Murray, Anal. Chem., 66, 682A (1994)

"Analytical chemistry provides the methods and tools needed for insight into our material world…for answering four basic questions about a material sample:

- What? (qualitative)
- Where? (spatial)
- How much? (quantitative)
- What arrangement, structure, or form? (speciation)

Federation of European Chemical Societies,
Karl Cammann, Univ. Muenster, 1992
Fresenius' Z. Anal. Chem., 343 (1992) 812

AMERICAN
CHEMICAL
SOCIETY

DIVISIONS
of
ANALYTICAL
CHEMISTRY

FEDERATION OF
EUROPEAN CHEMICAL
SOCIETIES

FIRST JOINT MEETING

EDUCATION IN ANALYTICAL CHEMISTRY

14-15 September 2001

CÓRDOBA, Spain

Some Highlights

- 5% of Western World’s economy dependent on analyses
- 20% of European chemists work as analysts
- 50% of chemists use analytical methods or results
- 3-5 billion pieces of analytical data/year in EU
- 100,000 analytical publications worldwide/year

60% of all legislation requires scientific input

Analytical chemistry provides measurements, leading to knowledge

Knowledge is the basis of democratic governance

Therefore, analytical chemistry is indispensible to governing a modern society

- **Manfred Grasserbauer**
  Director Joint Research
  Centre, European Commission

Some everyday tests that are important in our lives

- Blood glucose – diabetics
- Cholesterol levels
- Vitamin content of foods
- Pesticides in foods
- Carbon monoxide in air
- Auto emissions (CO, HC)

- Water hardness ($CaCO_3$)
- Nitrogen in fertilizer
- Sulfur in coal
- Carbon in steel
- Gunshot residue (forensics)
- Illicit drugs (criminal, sports)
- Rapid i.d. of toxic substances
- Chemical warfare agents

- **Health** (what is your cholesterol level?)
- **Safety** (does your food have pesticides?)
- **The environment** (what/who is polluting your water?)
- **Manufacturing** (real-time analysis, feedback control)
- **Quality control** (does the gasoline have the correct octane rating?)
- **Regulations** (do you meet emission requirements?)
- **Economic competitiveness** (increase yield, quality)
- **Forensics** (whose blood is it?)

How did analytical chemistry develop?

Perceived value of Au and Ag:

First incentive to acquire analytical knowledge.

Controlling purity and preventing counterfeiting was important in ancient communities in Babylon, Egypt, and Greece.

Fire Assays

"And I will put this third into the fire, and refine them as one refines silver, and test them as gold is tested."

Zechariah 13:9; Revised Standard Version

Fire Assays

King of Babylon complains to Egyptian Pharoah Amenophis the IVth (1375-1350 BC):

“Your majesty did not look at the gold sent to me. After putting it in the furnace, this gold was less than its weight.”

References to fire assay have been found on cuneiform tablets in the Babylonian language discovered in the Nile valley.

"There goes Archimedes with
his confounded lever again."

Chemical balance:

Ascribed to the Gods in the earliest documents found

Proverbs 11:l: “A false balance is an abomination to the Lord, but a just weight is his delight”

Art and science of weighing known in Egypt ca. 3000 B.C.

So measurements have always been important for societies.

And ethics/social responsibility have been issues over the eons,
and remain today.

More on this later.

Taiwan National Museum, Tapei

Han Dynasty 10 AD


新二鈞權 新六斤權 新三斤權 新銅丈

First Wet Test

1st Century – Pliny the Elder

(AD 23-79)

Caius Plinius Secundus
Roman author and philosopher
Natural History encylcopedia

Adulteration of copper sulfate was quite profitable.

Copper sulfate adulterated with iron sulfate - turned papyrus paper soaked in extract of gall-nuts black.

Middle Ages (470-1470)

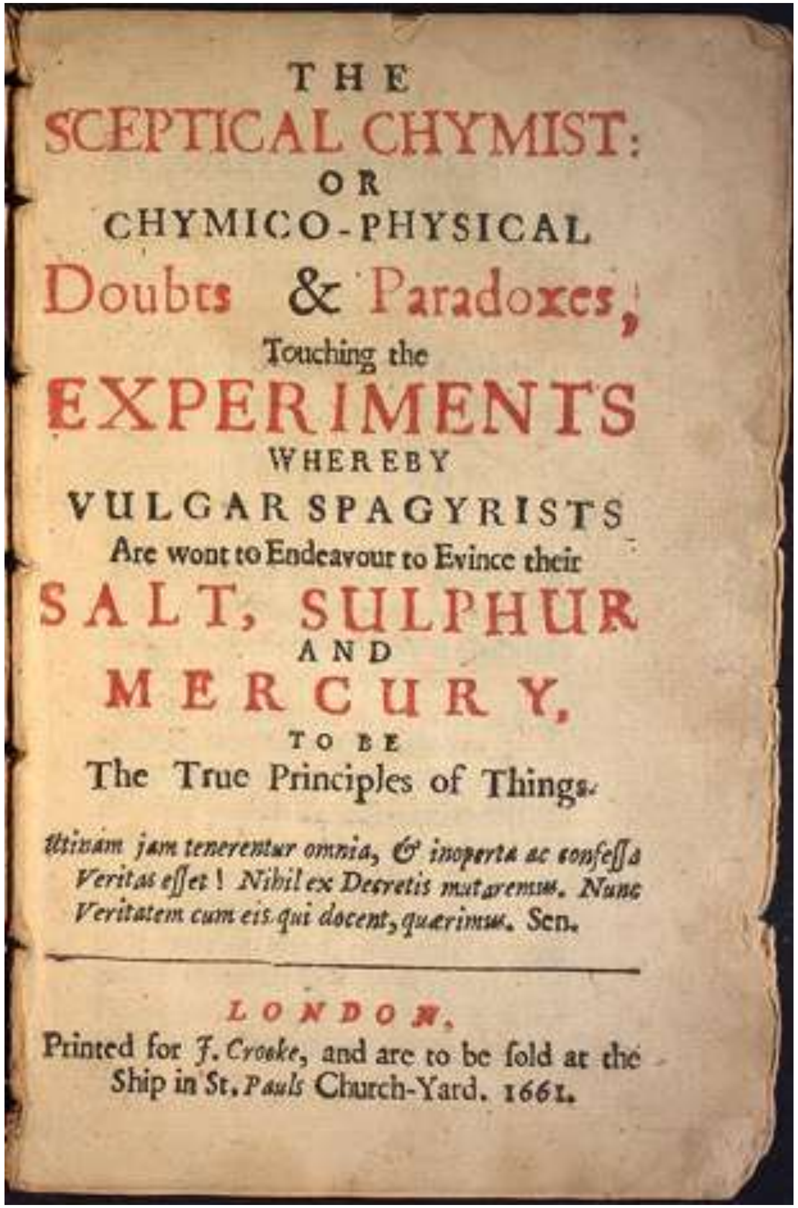
Alchemists – assembled knowledge that formed basis for quantitative analysis (3rd and 4th centuries)

Growth continued during the phlogiston era (to ~1700)

Robert Boyle
(1627-1691)

1661:
"The Sceptical Chymist"

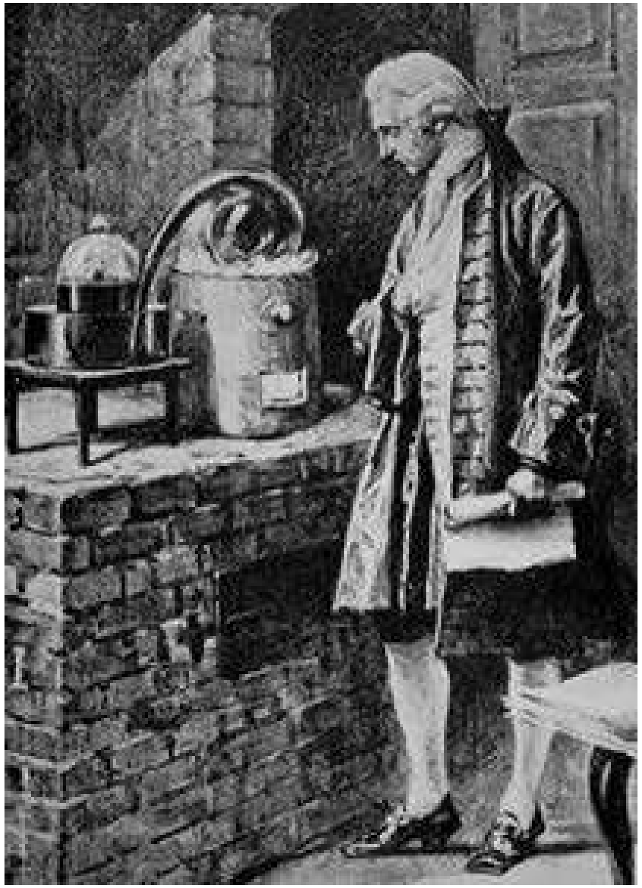
Coined the term "analyst"



THE
SCEPTICAL CHYMIST:
OR
CHYMICO-PHYSICAL
Doubts & Paradoxes,
Touching the
EXPERIMENTS
WHEREBY
VULGAR SPAGYRISTS
Are wont to Endeavour to Evince their
SALT, SULPHUR
AND
MERCURY,
TO BE
The True Principles of Things.

Utinam jam tenerentur omnia, & inoperta ac confeſſa Veritas eſſet! Nihil ex Decretis mutaremus. Nunc Veritatem cum eis qui docent, quærimus. Sen.

LONDON,
Printed for *J. Crooke*, and are to be ſold at the
Ship in St. *Pauls* Church-Yard. 1661.

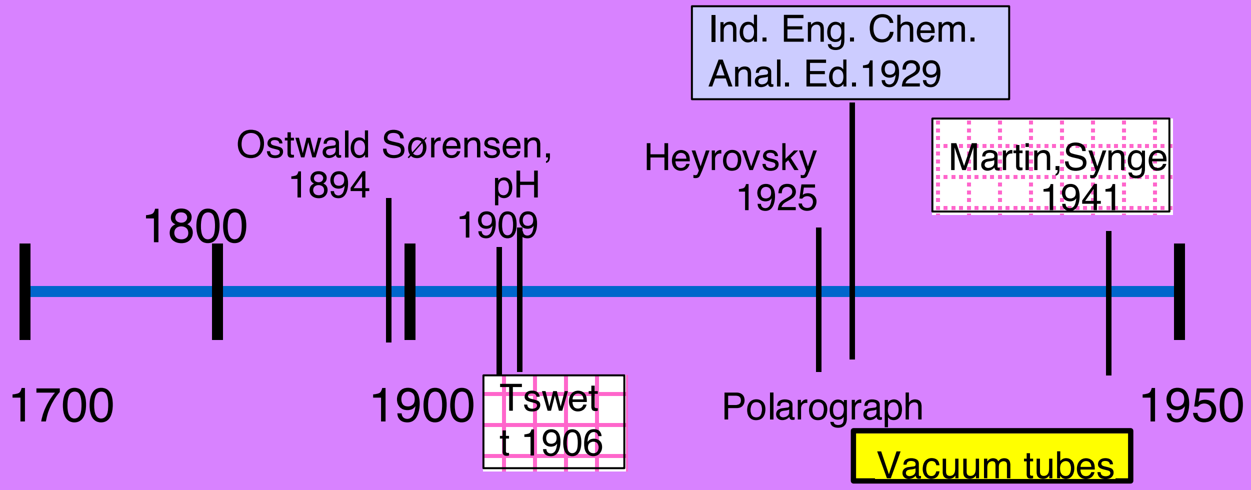


Antoine Lavoisier (1743-1794)

Antoine Lavoisier

The “father of quantitative analysis”

Used the balance for quantitative experiments on conservation of mass



Ind. Eng. Chem. Anal. Ed.1929

1800

Ostwald 1894

Sørensen, pH 1909

Heyrovsky 1925

Martin,Synge 1941

1700

1900

Tswett 1906

Polarograph

Vacuum tubes

1950

Gravimetric and titrimetric methods

Earliest instruments (e.g. visual colorimeters)

Introduction of physical chemistry concepts

Alan Bard, Pittcon 2002

Gravimetric Analysis – 17th Century

Friedrich Hoffmann (1660-1742)
(German physician-chemist)

Precipitated chlorides with silver nitrate and sulfates with lime

18th Century

Jons Jakob Berzelius (1779-1848)

-Introduced stoichiometric concepts

-Development of chemical microscopy, flame tests, bead tests, titrimetry

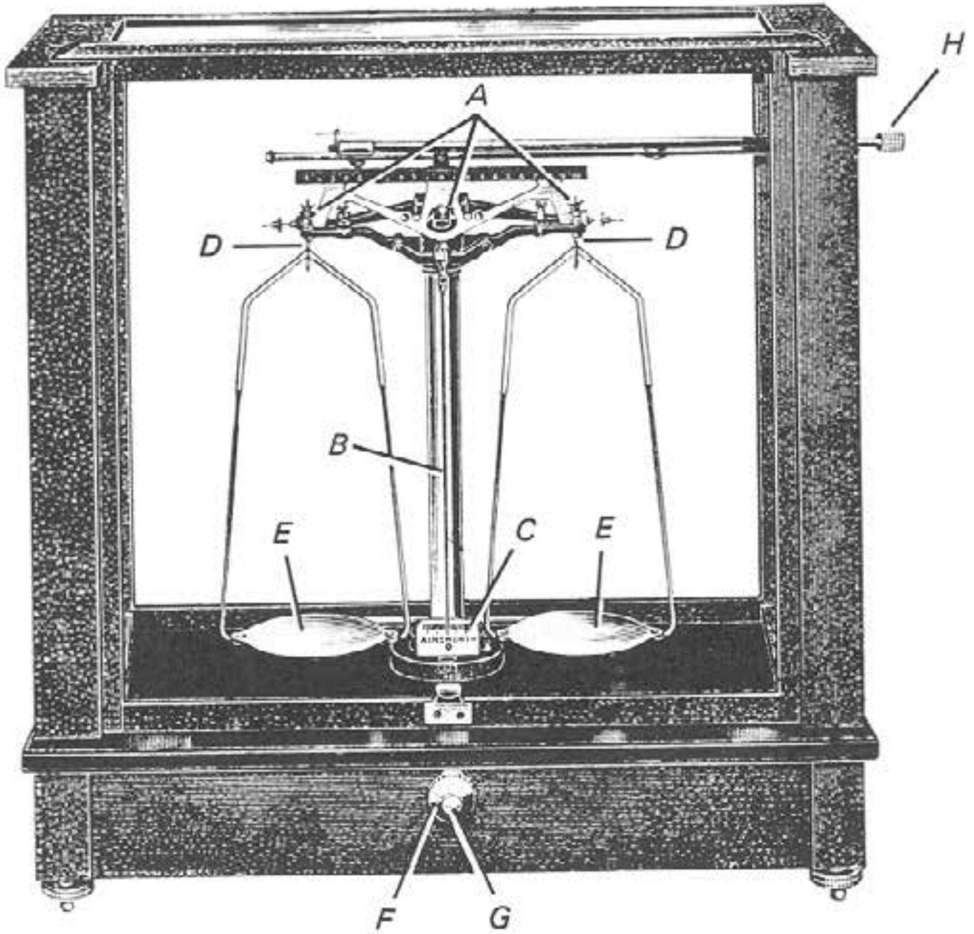
19th Century: Titrimetry

Bunsen

Robert Bunsen (1811-1899)
Karl Friedrich Mohr (1806-1879)

Joseph Gay-Lussac (1778-1850)
1829: Ag assay < 0.05% relative accuracy and precision
Designed the first burette
Named the burette and pipette

What tools do we use?


H
A
D
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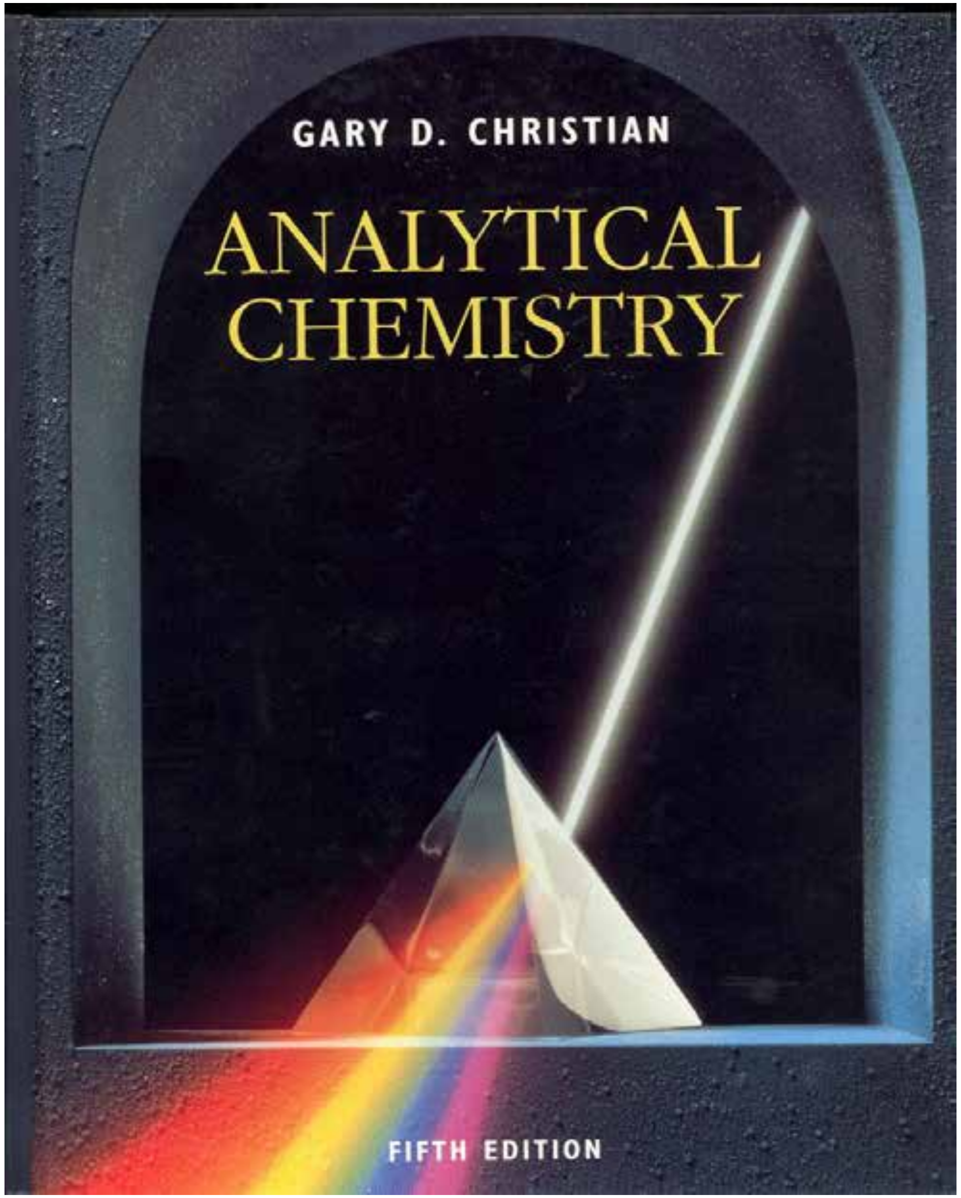
AINSWORTH
F
G

Modern balances are electronic. They still compare one mass against another since they are calibrated with a known mass. Common balances are sensitive to 0.1 mg.

Fig. 2.1. Electronic analytical balance.



GARY D. CHRISTIAN

ANALYTICAL CHEMISTRY

FIFTH EDITION

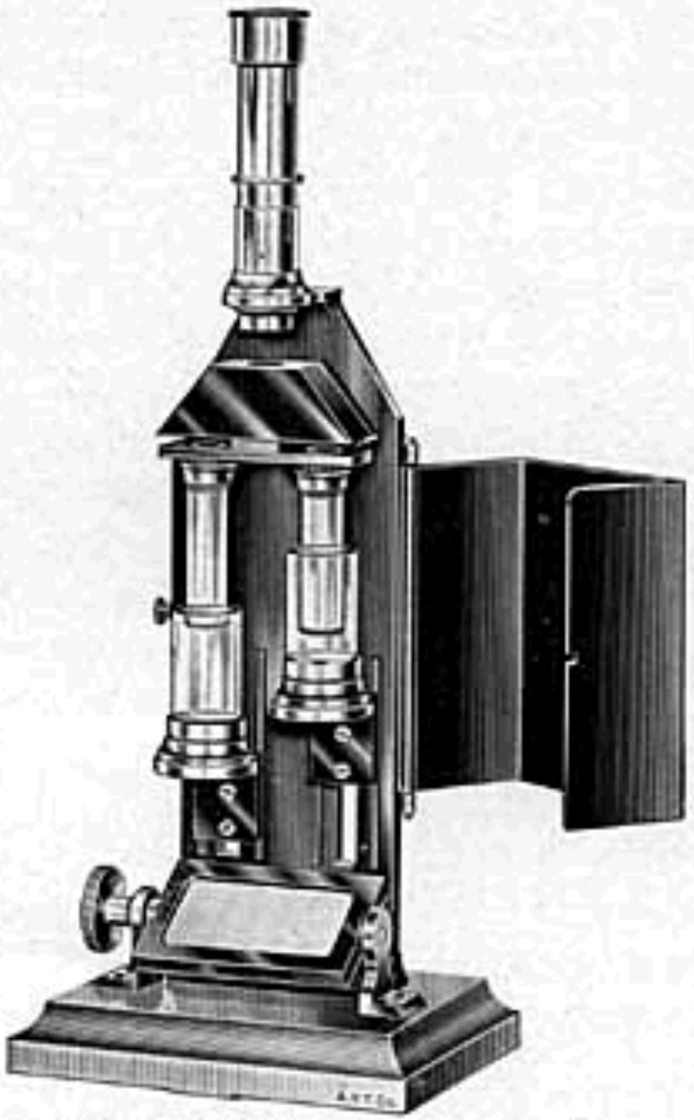
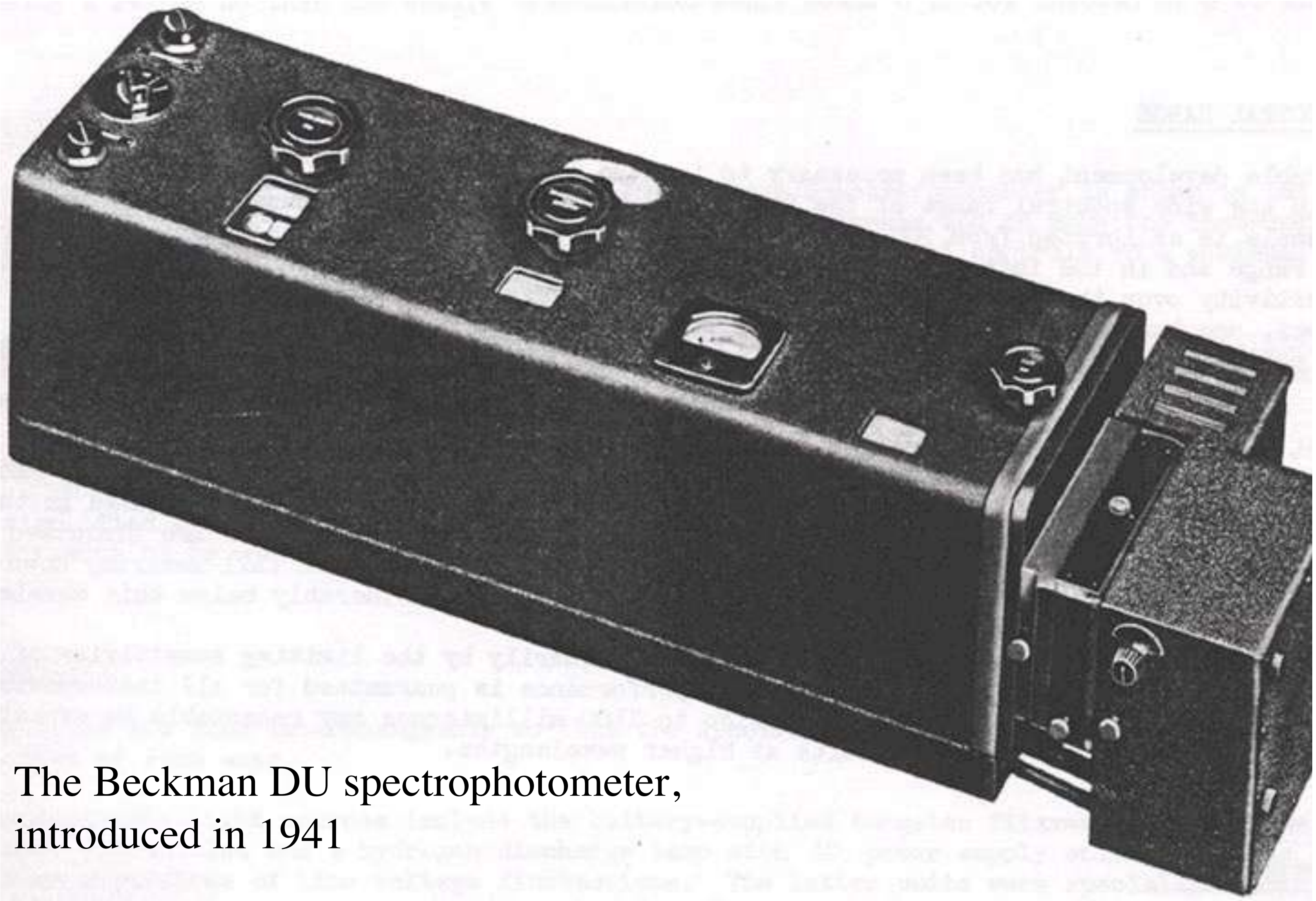


Fig. 25.—Duboscq colorimeter (Pellin).

Duboscq colorimeter (1854)

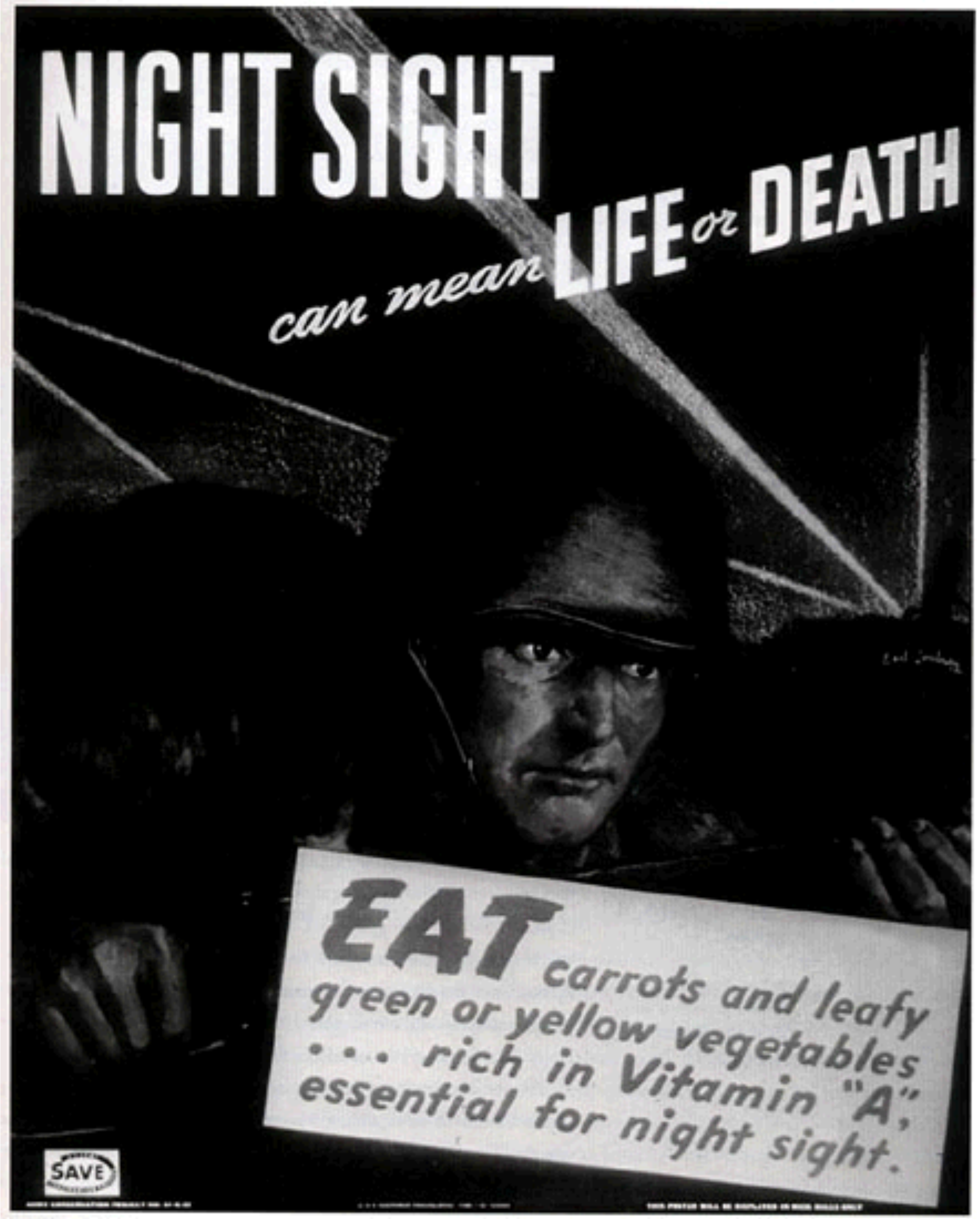
Used for the determination of creatinine in urine (Folin)

Alan Bard, Pittcon 2002



The Beckman DU spectrophotometer,
introduced in 1941

Alan Bard, Pittcon 2002



The pull for the invention of the Beckman DU was the need to measure vitamin A in food

Alan J. Bard, Pittcon 2002

Beckman Model G pH Meter
1936

Arnold O. Beckman
1900-2004

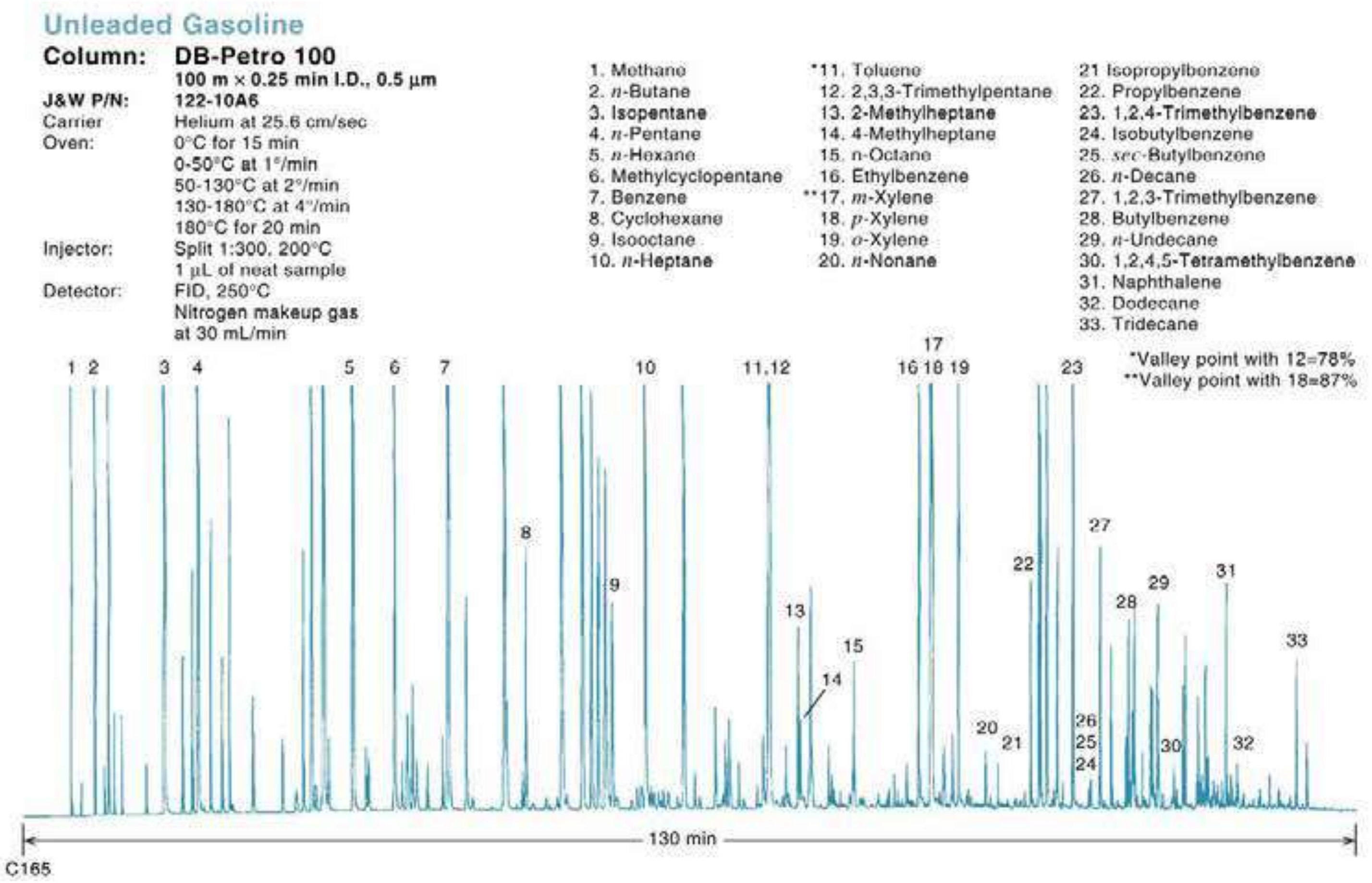
These include software for recording retention time, taking peak areas, and calculating concentrations.

An autosampler is attached.

Fig. 20.2. Modern gas chromatography system.

Hundreds of compounds can be separated and measured by GC, with very small samples.

Capillary columns have particularly high resolution.



Unleaded Gasoline

Column:	**DB-Petro 100** **100 m × 0.25 min I.D., 0.5 μm**
J&W P/N:	**122-10A6**
Carrier	Helium at 25.6 cm/sec
Oven:	0°C for 15 min 0-50°C at 1°/min 50-130°C at 2°/min 130-180°C at 4°/min 180°C for 20 min
Injector:	Split 1:300, 200°C 1 μL of neat sample
Detector:	FID, 250°C Nitrogen makeup gas at 30 mL/min

1. Methane
2. *n*-Butane
3. Isopentane
4. *n*-Pentane
5. *n*-Hexane
6. Methylcyclopentane
7. Benzene
8. Cyclohexane
9. Isooctane
10. *n*-Heptane

*11. Toluene
12. 2,3,3-Trimethylpentane
13. 2-Methylheptane
14. 4-Methylheptane
15. n-Octane
16. Ethylbenzene
**17. *m*-Xylene
18. *p*-Xylene
19. *o*-Xylene
20. *n*-Nonane

21 Isopropylbenzene
22. Propylbenzene
23. 1,2,4-Trimethylbenzene
24. Isobutylbenzene
25. *sec*-Butylbenzene
26. *n*-Decane
27. 1,2,3-Trimethylbenzene
28. Butylbenzene
29. *n*-Undecane
30. 1,2,4,5-Tetramethylbenzene
31. Naphthalene
32. Dodecane
33. Tridecane

*Valley point with 12=78%
**Valley point with 18=87%

Fig. 20.3. Typical gas chromatogram of complex mixture using a capillary column

©Gary Christian, Analytical Chemistry, 6th Ed. (Wiley)

GC-MS is very powerful for positive identification.

Modern GC-MS systems are compact.

More on principles in next slides.

Fig. 20.8. Gas chromatography-mass spectrometry benchtop system.

Top: Total-ion current gas chromatogram of cocaine in urine sample.

Middle: Mass spectrum from peak at 11.5 min.

Bottom: Mass spectrum from GC peak of cocaine standard at 11.5 min.

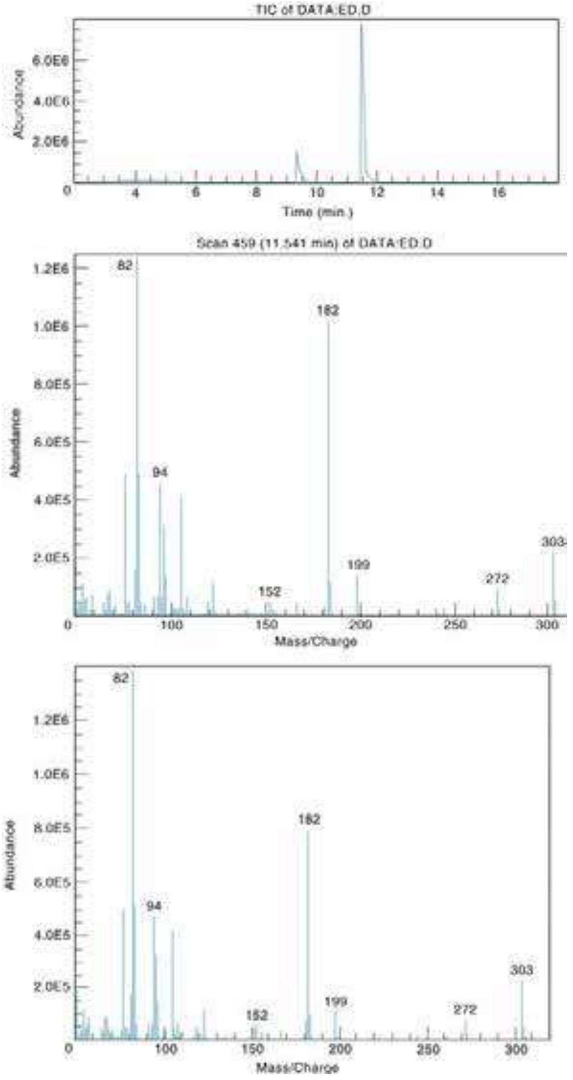


Fig. 20.13. Confirmation of cocaine by GC-MS.

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The evolution of textbooks

Karl F. Mohr (1808-1879):

“Lehrbuche der chemisch-analytischen Titrimethode” 1855 and 1856 (two parts)

Proposed primary standards
(oxalic acid for alkalimetry; ferrous ammonium sulfate for oxidimetry)

Used K_2CrO_4 indicator to improve Gay-Lussac’s turbidity method for chloride

Developed pinch clamp with a buret tip.

Introduced back titrations, normal solutions

Karl Remigius Fresenius
(1818-1897)

“Anleitung zur quantitativen chemischen Analyse,” 1846, 6 editions

1904 translation by A. I. Cohen
“Quantitative Chemical Analysis”

Founded Zeitschrift fur analytische Chemie 1862

Wilhelm Ostwald (1853-1932)

1894:

"Die wissenschaflichen Grundlagen der analytischem chemie"

"The scientific fundamentals of analytical chemistry"

Theoretical explanations of analytical phenomena, K_{eq}

“Analytical chemistry is doomed to continue occupying a position subordinate to other branches if analytical chemists do not stop teaching and practicing chemical analysis solely as an empirical technique and art”

Ostwald

1900-1939 period:

Gradual increase in emphasis on scientific approach vs. empirical approach.

E.g., formation and properties of precipitates (Kolthoff)

H. A. Laitinen
Talanta, **36**, 1 (1989)

Textbook archeology (Royce Murray)

1930-1950: Basic chemical reactivity and physical aspects of titrimetry and gravimetry (Kolthoff and Sandell)

1960’s: Spectrophotometry, separations, electrochemistry, gravimetry decreased

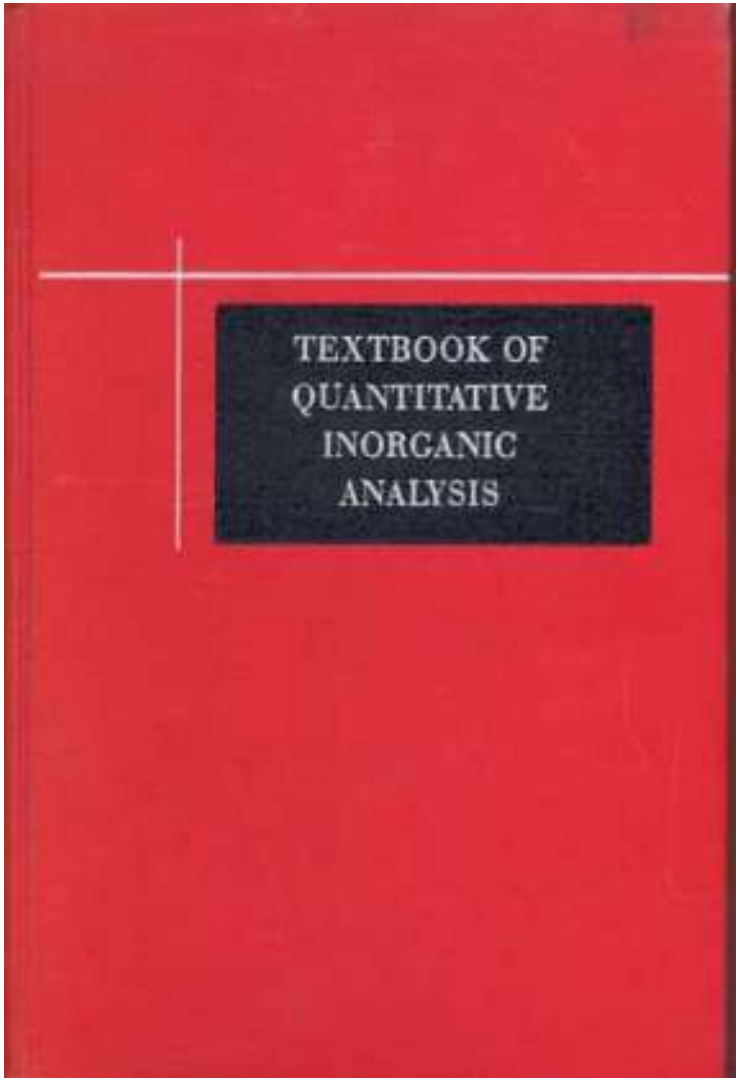
Titrimetry constant over 40 years. But:

Quant. treatment of equilibria
Reactivity
Electrode potentials

(1894-1993)

I. M. Kolthoff and E. B. Sandell, 1936:

“Textbook of Quantitative Inorganic Analysis”



TEXTBOOK OF
QUANTITATIVE
INORGANIC
ANALYSIS

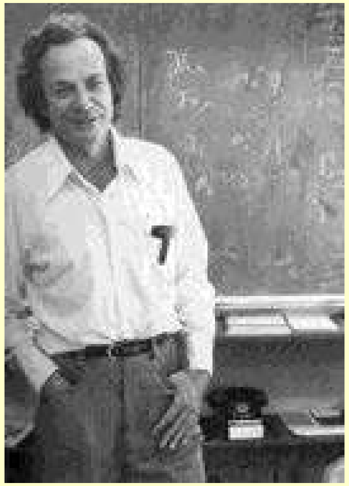
“There appears to be a tendency to exaggerate the significance of “theory” at the expense of practical work in chemical analyses.”

Kolthoff and Sandell, 1936

“Theory guides, experiment decides.”

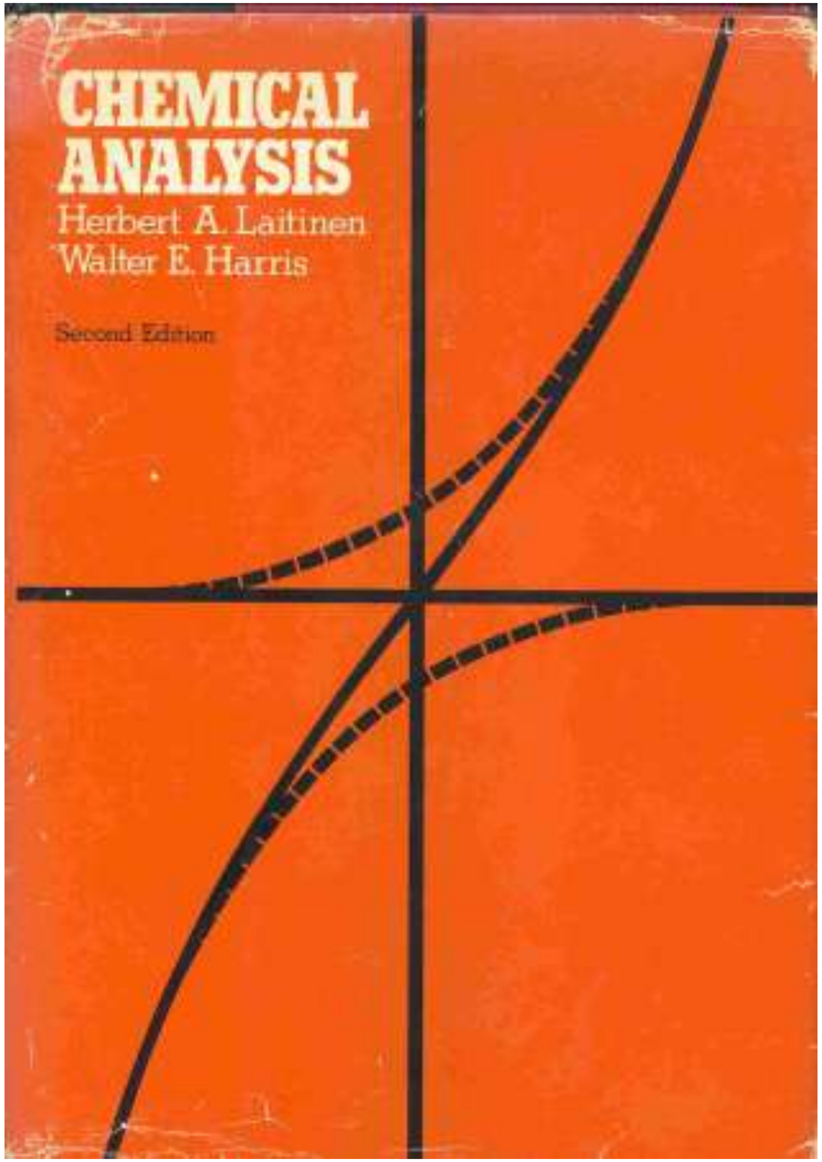
I. M. Kolthoff

Boyle: “Theory must be supported by experiment”
- 1661



Richard P. Feynman, 1918-1988

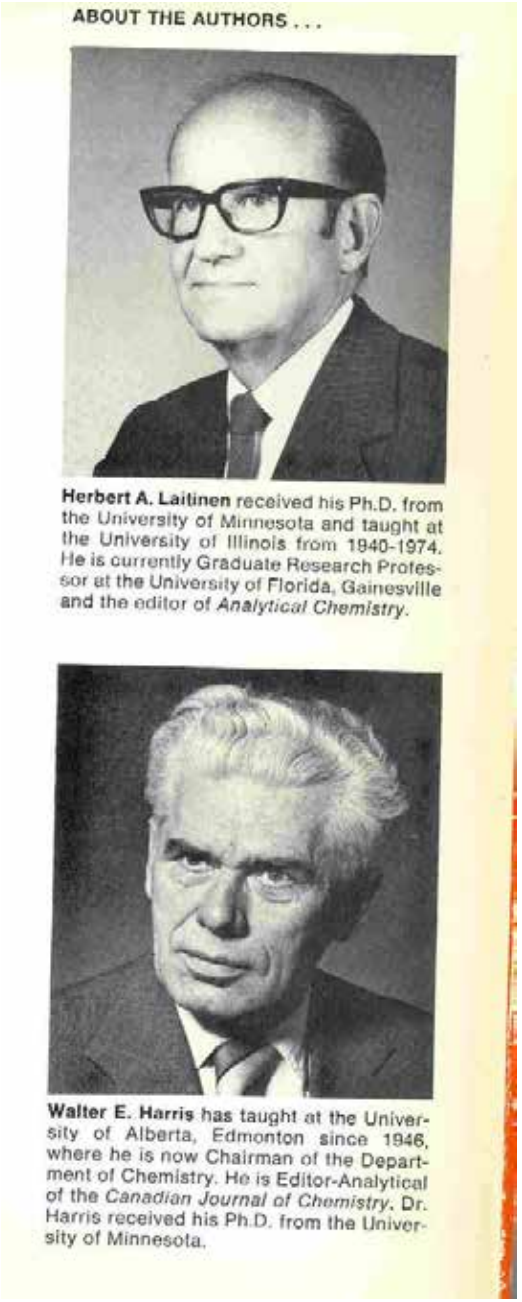
“The test of all knowledge is experiment”



CHEMICAL ANALYSIS
Herbert A. Laitinen
Walter E. Harris

Second Edition

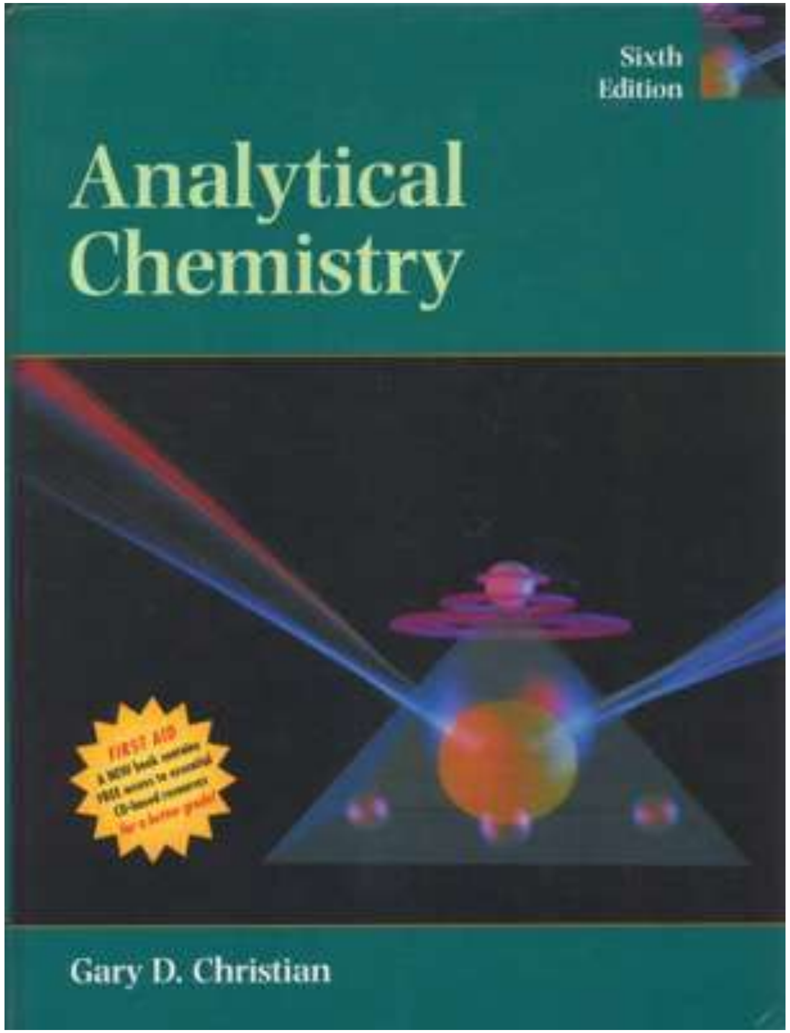
1st ed. 1960   2nd ed. 1975



ABOUT THE AUTHORS . . .

Herbert A. Laitinen received his Ph.D. from the University of Minnesota and taught at the University of Illinois from 1940-1974. He is currently Graduate Research Professor at the University of Florida, Gainesville and the editor of *Analytical Chemistry*.

Walter E. Harris has taught at the University of Alberta, Edmonton since 1946, where he is now Chairman of the Department of Chemistry. He is Editor-Analytical of the *Canadian Journal of Chemistry*. Dr. Harris received his Ph.D. from the University of Minnesota.



Sixth
Edition

Analytical
Chemistry

Gary D. Christian

Validation involves determining:

- **selectivity**
- **linearity**
- **accuracy**
- **precision**
- **sensitivity**
- **range**
- **limit of detection**
- **limit of quantitation**
- **ruggedness/robustness**

Standard reference materials (SRMs) best for determining accuracy.

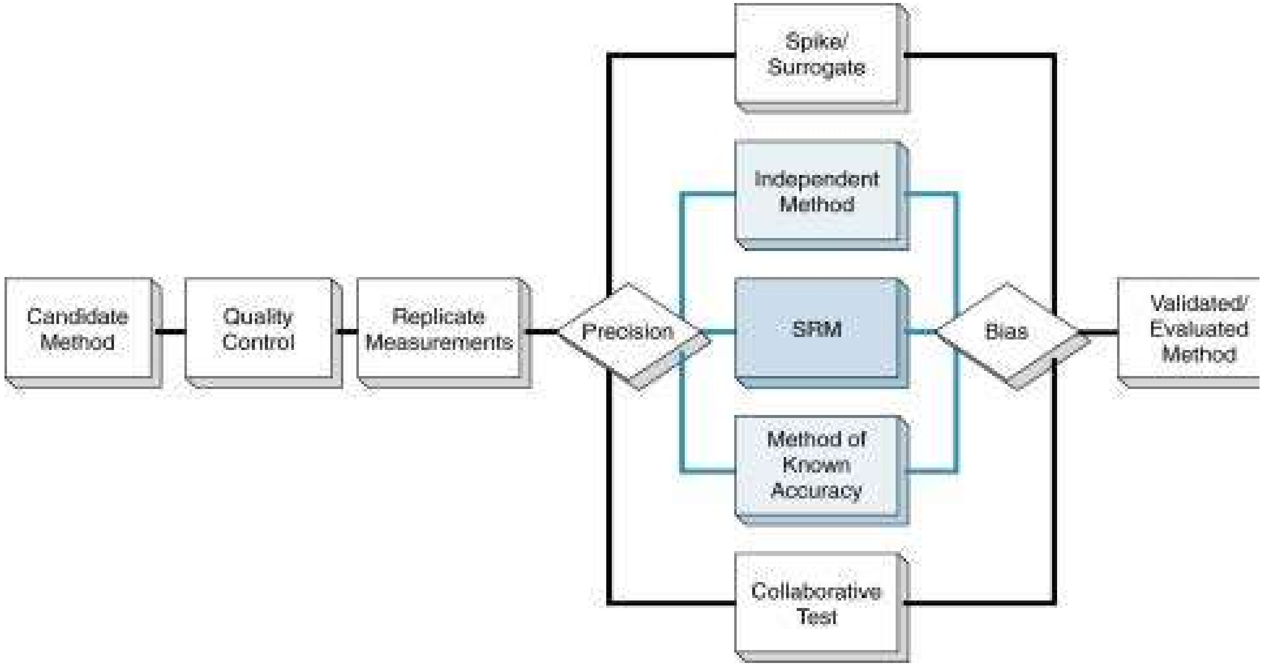
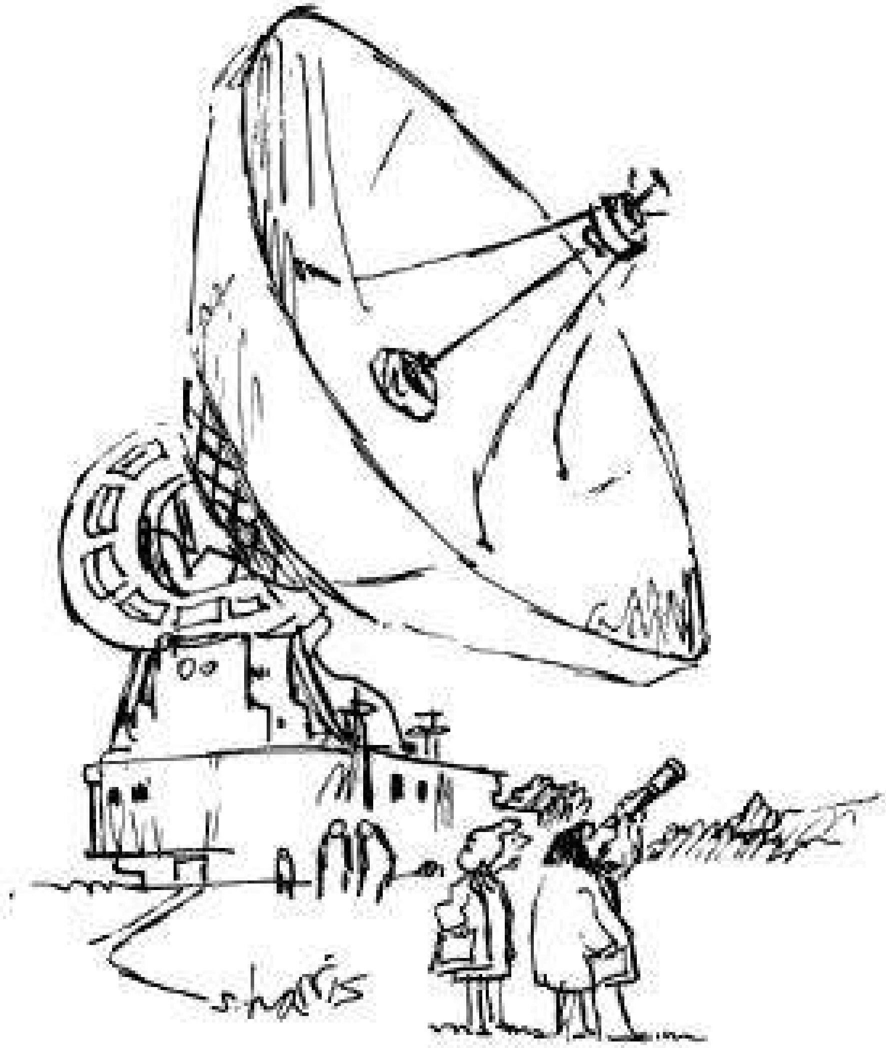


Fig. 4.1. General process for evaluation/validation of methodology



"Just checking."

Bases are separated in order of size.

Each band in a lane has one of the four base colors.

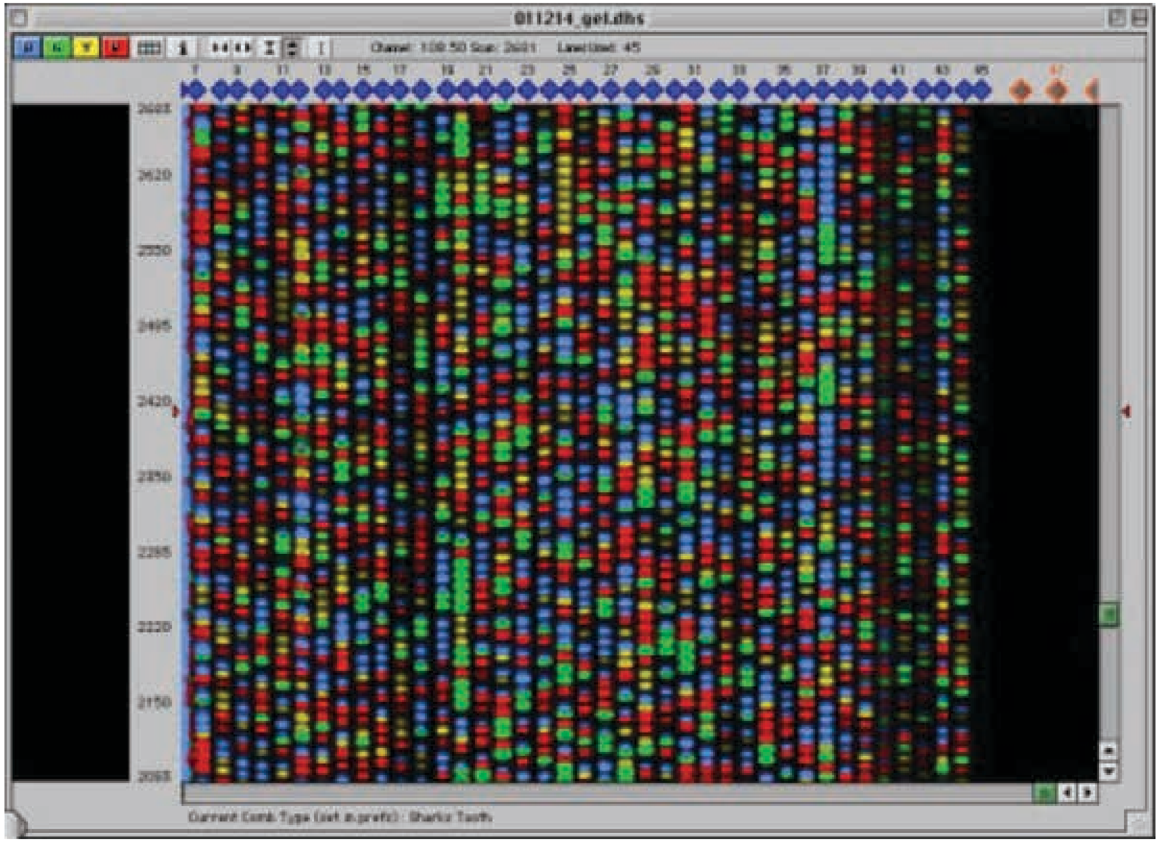


Fig. 25.9. Gel electrophoresis separation of nucleotides. Each vertical lane represents a different sample.

Proteins perform most of life functions.

Protein structure needs to be understood to understand function.

Proteomics is the study of proteins in the cell:

- **protein sequencing to determine structure**
- **protein interaction**

We study the expression of genes in producing proteins.

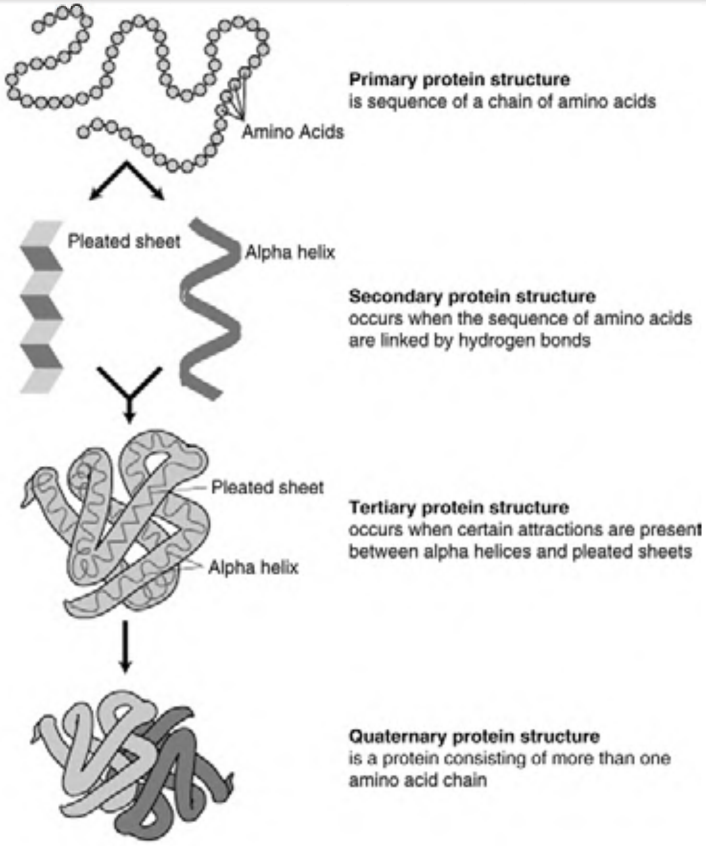


Fig. 25.11. Protein structure.

In 2-D PAGE (polyacrylamide gel electrophoresis), proteins are first separated based on charge.

Then they are separated based on size to give a 2-D plot.

Proteins in individual spots are excised, degraded into a mixture of peptides,
and analyzed by MALDI-TOF (mass spectrometry).

Computer databases identify the protein form the peptide sequences.

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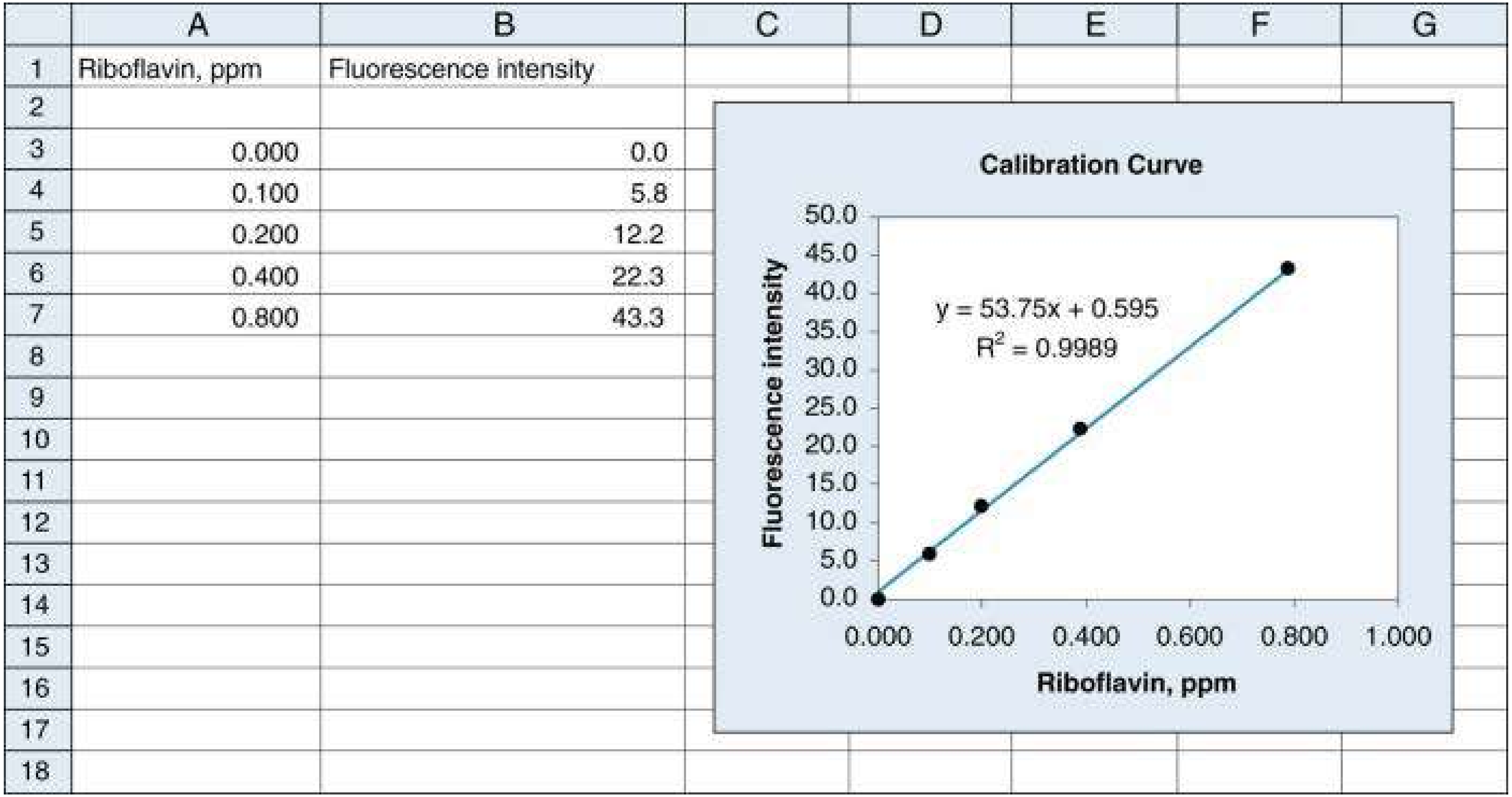
Analytical Chemistry,
6th Ed. (Wiley)

Fig. 25.12. 2D-gel separation of proteins.

You may insert the graph within the data sheet (Sheet 1), or a new Sheet 2.



	A	B	C	D	E	F	G
1	Riboflavin, ppm	Fluorescence intensity					
2							
3	0.000	0.0					
4	0.100	5.8					
5	0.200	12.2					
6	0.400	22.3					
7	0.800	43.3					
8							
9							
10							
11							
12							
13							
14							
15							
16							
17							
18							

Fig. 3.9. Calibration graph inserted in spreadsheet (Sheet 1).

What is taught?

In the U.S., there is no set curriculum

Each department in a university sets the curriculum

Some stick to standard curriculum

Others have deleted or downgraded older methodologies like gravimetry or titrimetry in favor of those more used in the real world

But some value the basics and rigor of the standard methods. In the laboratory, they teach care in measurement.

Teaching equilibria is always a challenge, but considered important in many fields. Spreadsheets can help students.

1980 Symposium on Teaching of Analytical Chemistry

Survey of 25 major institutions:

40% taught analytical chemistry in Freshman year
- Some by analytical chemists
- Some by others, and only lab

Typical texts:
- Gravimetry
- Volumetric methods
- Acid-base equilibria
- Spectrophotometry (UV-vis, IR, atomic)
- Potentiometry
- Separations (solvent extraction, chromatography)

1984 ACS Exam Survey

175 schools solicited, 95 responses
List of 100 topics:
Not one topic was checked 100% of time

Top 30%:
- General classical methods
- Statistics
- Potentiometry
- Spectrophotometry

Next 10%:
- Atomic spectrometry
- Chromatography

Lower 50%:
- Instrumental topics:
  - voltammetry, IR

Peter Griffiths, University of Idaho, 2007

Survey of Universities in the Western USA

(Society of Western Analytical Professors Mailing List)

Do you use the ACS Examination?

How many lecture periods on different topics?

Is this topic covered in the laboratory?

Peter Griffiths, 2007

Who Takes The Course?

Major Subject	% of Respondents
Chemistry majors and minors	70%
Biochemistry majors	15%
Others include: •Chemical engineering •Microbiology, molecular biology •Food science, nutrition •Environmental studies •Industrial hygiene, public health •Geology •Medical technology •Forensic anthropology	15%

Peter Griffiths, 2007

Topics and Percentage Not Covered

Solution Preparation	43%
Error analysis and statistics	0%
Sampling	53%
Spread sheets	63%
Equilibria	3%
Activity	13%
Titration curves (general)	17%

Peter Griffiths, 2007

Topics and Percentage Not Covered

Acid-base equilibria	3%
Acid-base titrations	7%
Buffer solutions	13%
Precipitation equilibria	23%
Precipitation titrations	60%
Gravimetric analysis	50%
Complexometric titrations	33%

Peter Griffiths, 2007

Topics and Percentage Not Covered

Reduction and oxidation	10%
Redox titrations	27%
Potentiometry	17%
Coulometry	53%
Other electrochemical methods	60%

Should these be covered in a future instrumental analysis course?

Peter Griffiths, 2007

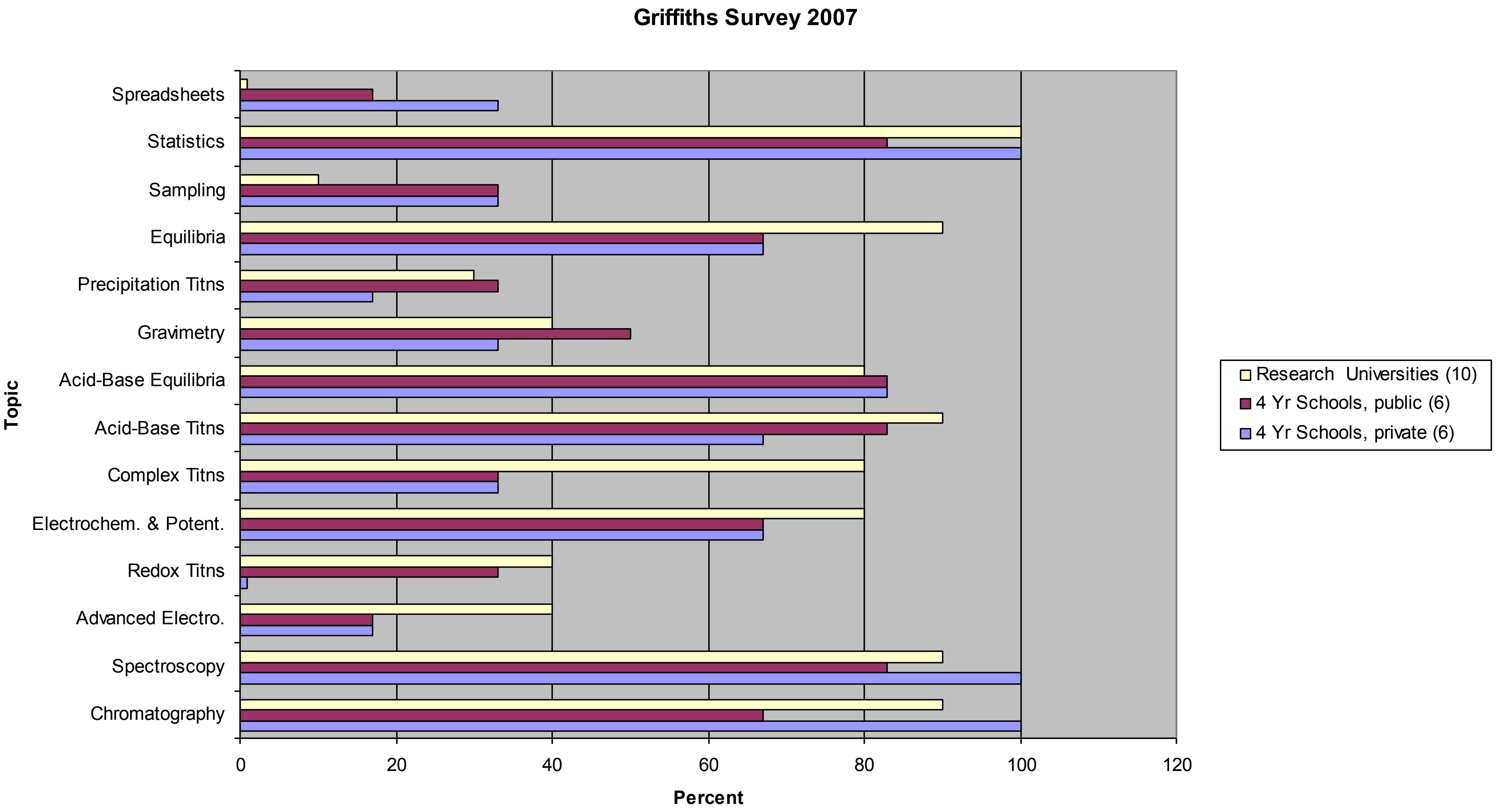
Topics and Percentage Not Covered

Separation and chromatography theory	13%
Gas chromatography	30%
HPLC	40%

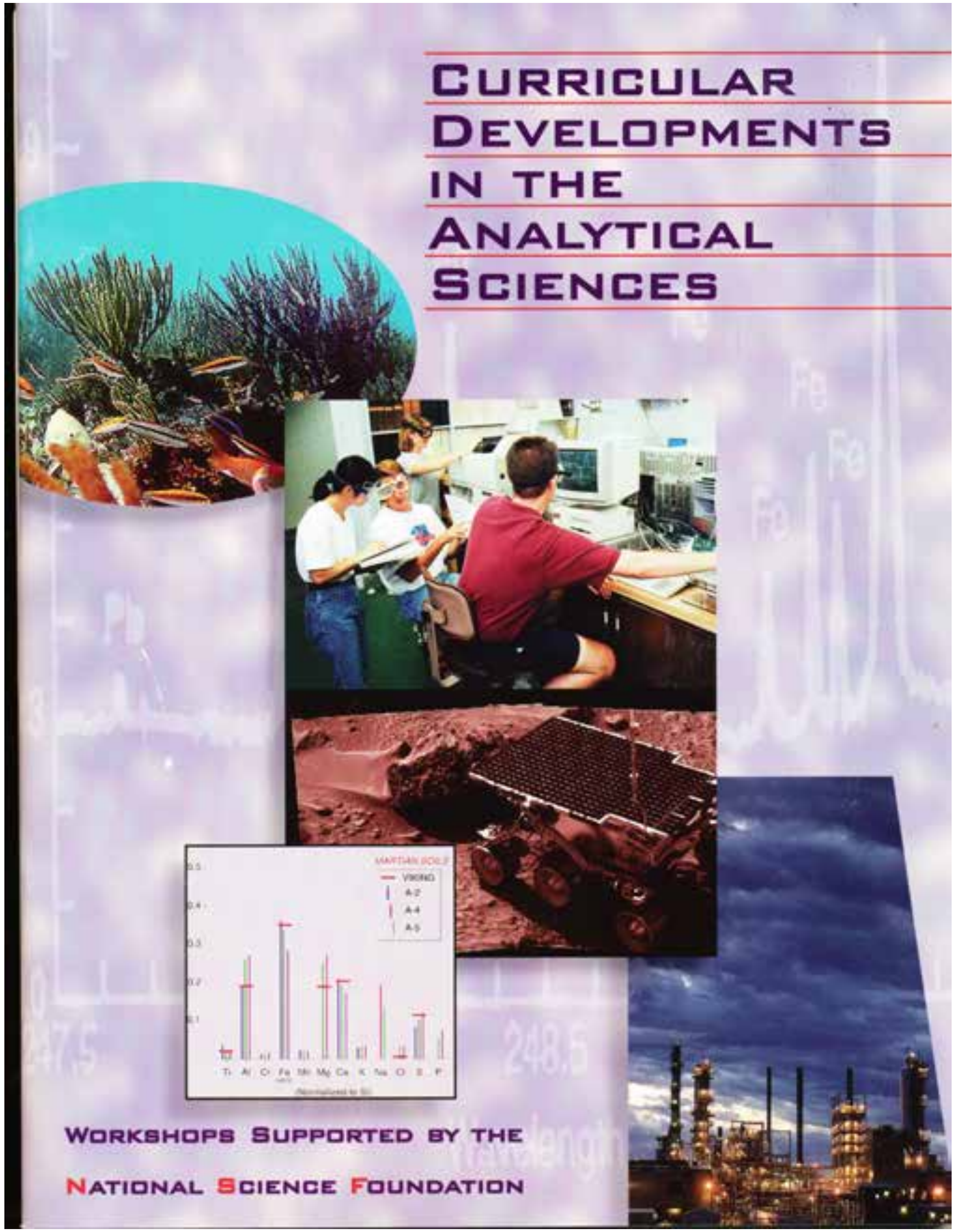
Electrophoresis	80%
Ion exchange	77%

Should these be covered in a future instrumental analysis course?

Peter Griffiths, 2007



Peter Griffiths, 2007



CURRICULAR DEVELOPMENTS IN THE ANALYTICAL SCIENCES

WORKSHOPS SUPPORTED BY THE

NATIONAL SCIENCE FOUNDATION

1997 Report

http://www.asdlib.org/files/curricularDevelopment_report.pdf

CURRICULAR DEVELOPMENTS IN THE ANALYTICAL SCIENCES

A Report from the Workshops

October
28-30, 1996
Leesburg, VA

March 13-15, 1997
Atlanta, GA

SUMMARY OF RECOMMENDATIONS AND IMPLEMENTATION MODES

1 . COURSE CONTENT AND LEARNING MODES

Undergraduate analytical curricula need to better prepare students to solve future problems and to pursue analytical science careers.

1 . COURSE CONTENT AND LEARNING MODES

RECOMMENDATION 1

That the analytical community develop context-based curricula that incorporate problem-based learning (PBL)

Students must know how to use the scientific method & the analytical process

To be effective, must encompass:

- **Complete process sampling**
- **Sample preparation or separation**
- **Measurement**
- **Data analysis and interpretation**

1 . COURSE CONTENT AND LEARNING MODES

RECOMMENDATION 2

That teaching styles accommodate students' different learning needs.

Methods should emphasize the development of oral and written communication skills:

- **Small-group learning**
- **Cooperative learning**
- **Project-centered classes**
- **Investigative-oriented labs and lectures**
- **Case studies**
- **Emerging technologies**
- **Assessment tools of context-based leaning**

1 . COURSE CONTENT AND LEARNING MODES

RECOMMENDATION 3

That more students be offered hands-on learning opportunities.

Bring **context-based learning** to introductory courses

Context-based educational principles should be used in the **introductory chemistry labs that involve analytical measurements**.

Provide **undergraduates research opportunities** with faculty members

2. CORE TECHNOLOGIES FOR UNDERGRADUATE LABS

RECOMMENDATION 1

That the analytical community develop a list of appropriate and well developed technologies that faculty may consider for their classes and laboratories.

Pursue continuing education: Faculty must actively upgrade their technological skills

Encourage vendors to serve the education market

Broaden definition of technology: By broadening the definition of technology to include more than what might be found in analytical chemistry

2. CORE TECHNOLOGIES FOR UNDERGRADUATE LABS

RECOMMENDATION 2

That faculty and their departments strive to incorporate today’s technology into classrooms and laboratories and to use technology as an access to real-world leaning.

Use technology to link classrooms and to enhance learning: Through the Internet, the web, video-teleconferencing, and virtual classrooms and laboratories

3. FACULTY DEVELOPMENT

RECOMMENDATION: **That faculty in the analytical areas broaden their technical skills and industry awareness by seeking non-academic resources and learning opportunities.**

- **Invite non-academics to campus**

- **Seek sources for real-world problems**

  Through contacts with local and regional industries, faculty can find sources for real-world problems and even samples that can be usedin the classroom and laboratory.

- **Develop exchange and visitation programs**

- **Establish a non-academic advisory board**

- **Support development of the Senior Analytical Corps**

4. LEARNING PARTNERSHIPS WITH INDUSTRY

RECOMMENDATION

That industries form learning partnerships with educators in the analytical sciences.

European Credit Transfer and Accumlation System

:: What is:

Credit system

A credit system is a systematic way of describing an educational programme by attaching credits to its components.

The definition of credits in higher education systems may be based on different parameters, such as student workload, learning outcomes and contact hours.

ECTS

The European Credit Transfer and Accumulation System is a student-centred system based on the student workload required to achieve the objectives of a programme, objectives preferably specified in terms of learning outcomes and competences to be acquired.

How did ECTS develop?

ECTS was introduced in 1989, within the framework of Erasmus, now part of the Socrates programme. ECTS is the only credit system which has been successfully tested and used across Europe. ECTS was set up initially for credit transfer.

The system facilitated the recognition of periods of study abroad and thus enhanced the quality and volume of student mobility in Europe. Recently ECTS is developing into an accumulation system to be implemented at institutional, regional, national and European level.

This is one of the key objectives of the Bologna Declaration of June 1999.

Regarding the minimum content in Analytical Chemistry for all Spanish Universities, there is the “White Book of the Degree in Chemistry” edited by ANECA (National Agency for Quality Evaluation and Accreditation). It is in Spanish (204 pages)

This document fixes a minimum content of 22.5 ECTS for Analytical Chemistry.

Minimum content of 22.5 ECTS for Analytical Chemistry.
The minimum theoretical content is as follows:

- The analytical process
- The measurement in Analytical Chemistry
- Analytical Chemistry of solutions
- Qualitative analysis: identification of chemical species
- Gravimetric and volumetric quantitative analysis
- Analytical separation techniques: non chromatographic and chromatographic techniques
- Instrumental analysis: general principles-Optical techniques of analysis
- Optical techniques of analysis
- Electroanalytical techniques
- Instrumental hybridation
- Introduction to chemometrics

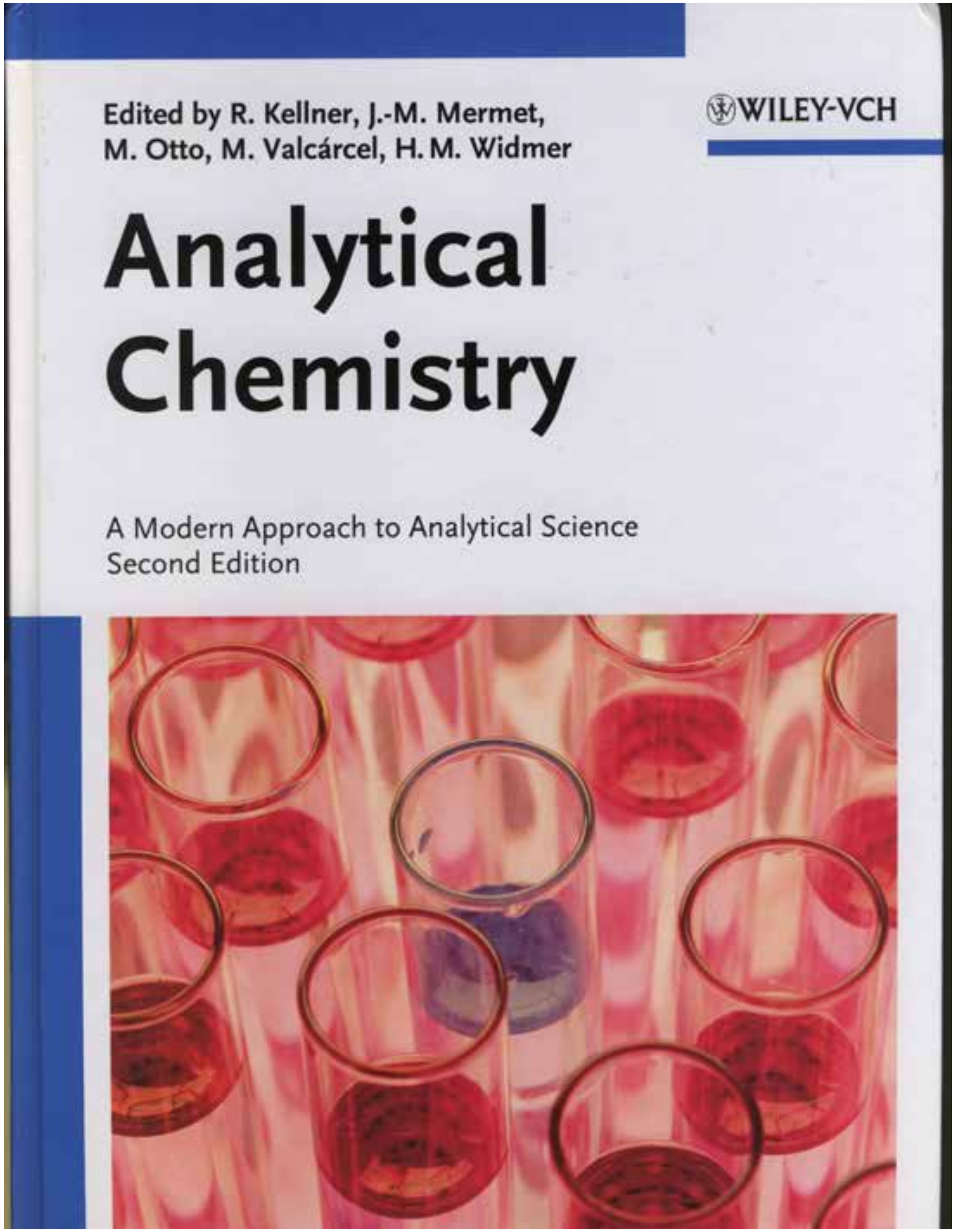
The document also suggests the distribution of the minimum theoretical content and the practical content into three parts:

- **Analytical Chemistry I** (The analytical process, The measurement in Analytical Chemistry, Analytical Chemistry of solutions, Qualitative analysis: identification of chemical species, Gravimetric and volumetric quantitative analysis). Minimum 5 theoretical ECTS plus 2.5 practical ECTS.
- **Analytical Chemistry II** (Analytical separation techniques: non chromatographic and chromatographic techniques, Instrumental analysis: general principles, Optical techniques of analysis, Electroanalytical techniques, Instrumental hybridation, Introduction to chemometrics). Minimum 10 theoretical ECTS.
- **Experimental Analytical Chemistry** (Applications of the main instrumental techniques: non chromatographic and chromatographic techniques, optical techniques of analysis, electroanalytical techniques, etc.). Minimum 6 practical ECTS.

Of course, there are some differences among universities.

For instance, the University of Salamanca decided to split Analytical Chemistry II into two subjects:

- One for separations techniques (6 ECTS)
- Another one for instrumental analysis (6ECTS).
- This makes a total of 12 ECTS (two more than the minimum fixed in the White Book).



Edited by R. Kellner, J.-M. Mermet,
M. Otto, M. Valcárcel, H. M. Widmer

WILEY-VCH

Analytical Chemistry

A Modern Approach to Analytical Science
Second Edition

Quantitative Analysis Experiments, U.W.

Safety, Volumetric glassware use, Weighing operations, Lab notebook

1. Gravimetric determination of chloride

2. pH titration of unknown weak base

3. EDTA titration of calcium (H_2O hardness)

4. Iodometric determination of ascorbic acid

5. Potentiometric determination of F^- in H_2O

6. Spectrophotometric determination of manganese by standard addition method

7. Solid phase extraction/preconcentration and spectrophotometric determination of methyl red

8. Reaction rate assay of glucose

9. Ion chromatography (mixture of Cl^- & NO_3^-)

Instrumental Analysis Experiments, U.W.

1. Separation of Common Analgesics by HPLC
(salicylamide, Tylenol, caffeine, aspirin)

2. Capillary GC-MS

3. Cyclic Voltammetry (ferricyanide reduction)

4. Determination of Fat Content of Milk by FTIR

5. Flow Injection Analysis (D, throughput, Al in H_2O)

6. Determination of Metals by Plasma Emission

Some New Ways We Teach – Modern Technology

We have new ways to interact with students and to deliver to them:

PowerPoint
Email
Text message
Posting lectures, problems
Answering them
etc. etc.

I’m glad I don’t have to keep up with all of this now.

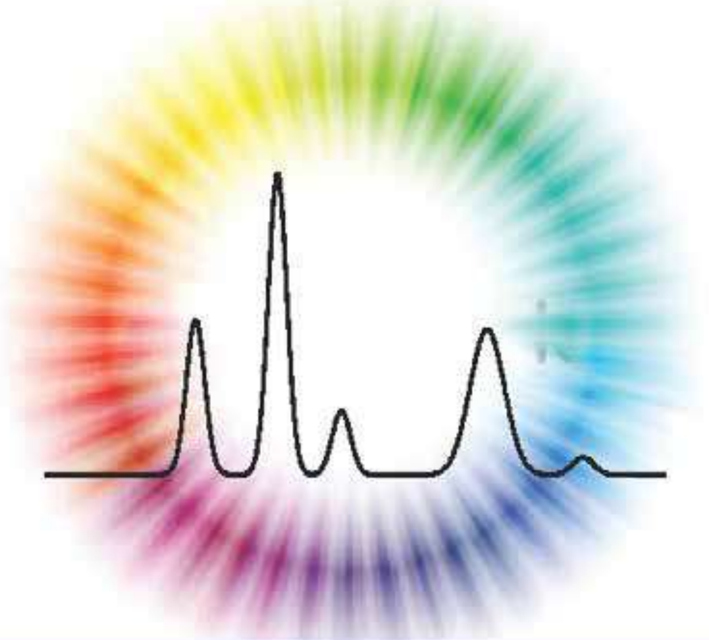
And it surely takes more of the instructor’s time.
Example: Sandy Dasgupta spreadsheet problems, videos

Spreadsheets allow us to perform complicated calculations, plots

- Titration curves, derivatives
- Alpha vs. pH plots
- log C vs. pH plots
- Equilibrium calculations

Seventh Edition

ANALYTICAL CHEMISTRY



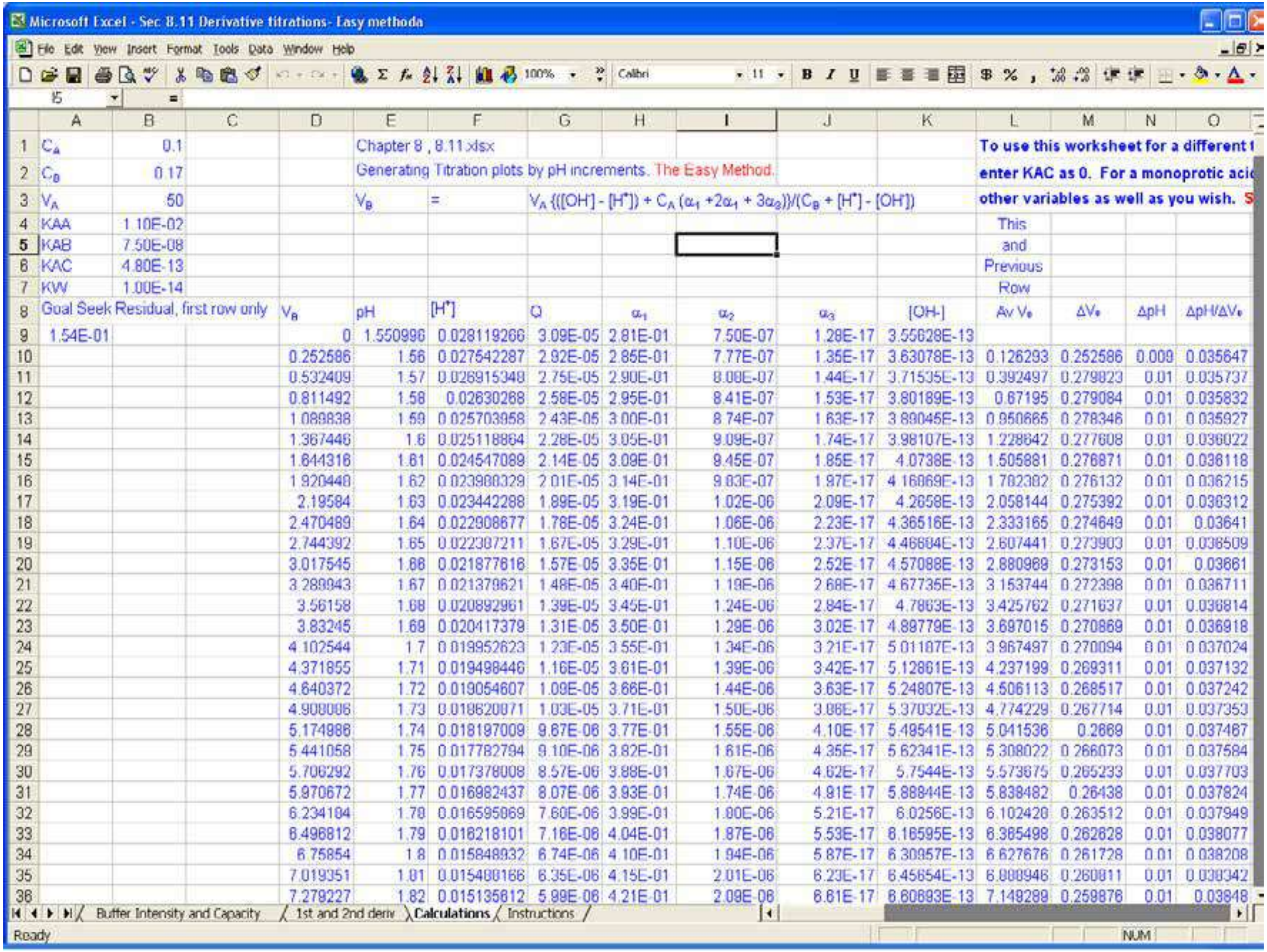
Gary D. Christian • Purnendu K. Dasgupta • Kevin A. Schug

WILEY

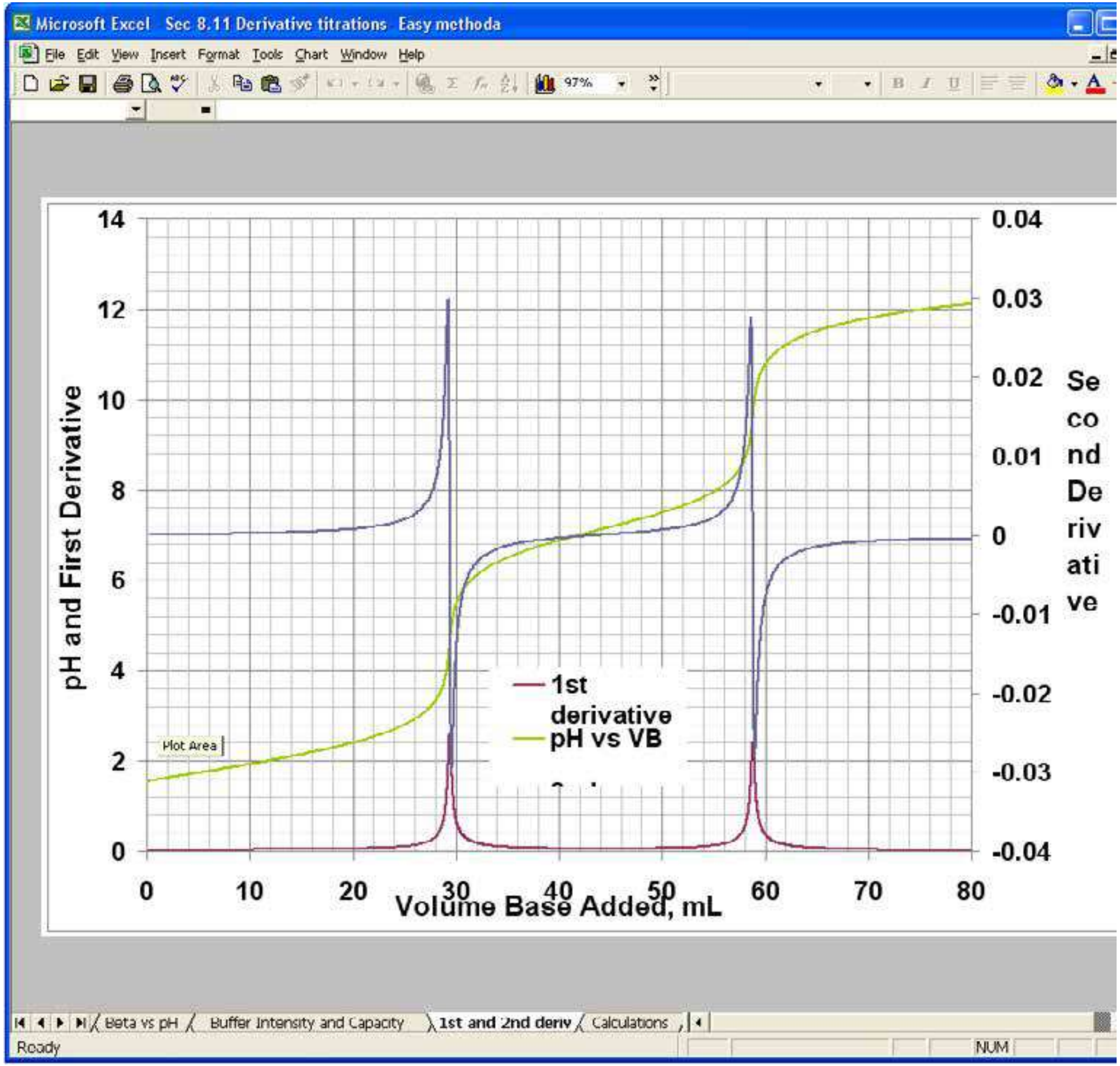
Reviewer biggest challenges:

- While students do well in lab, understanding theory behind the techniques & solving analytical problems are their biggest hurdles
- Many concepts have to be retaught: relearning concepts like equilibrium
- Wide range in academic ability & background
- Weak math skills
- Challenge students to think critically vs. cookbook thinking
- Finding a balance between breadth & depth

Derivative titration curves – H_3PO_4 titration



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	C_A	0.1			Chapter 8 , 8.11.xlsx							To use this worksheet for a different t			
2	C_B	0.17			Generating Titration plots by pH increments. The Easy Method.							enter KAC as 0. For a monoprotic aci			
3	V_A	50			V_B	=	$V_A \{(([OH^-] - [H^+]) + C_A(\alpha_1 + 2\alpha_1 + 3\alpha_3)\}/(C_B + [H^+] - [OH^-])$					other variables as well as you wish. S			
4	KAA	1.10E-02										This			
5	KAB	7.50E-08										and			
6	KAC	4.80E-13										Previous			
7	KW	1.00E-14										Row			
8	Goal Seek Residual, first row only			V_B	pH	$[H^+]$	Q	α_1	α_2	α_3	[OH-]	Av V_B	ΔV_B	ΔpH	$\Delta pH/\Delta V_B$
9	1.54E-01			0	1.550996	0.028119266	3.09E-05	2.81E-01	7.50E-07	1.28E-17	3.55628E-13				
10				0.252586	1.56	0.027542287	2.92E-05	2.85E-01	7.77E-07	1.35E-17	3.63078E-13	0.126293	0.252586	0.009	0.035647
11				0.532409	1.57	0.026915348	2.75E-05	2.90E-01	8.08E-07	1.44E-17	3.71535E-13	0.392497	0.279823	0.01	0.035737
12				0.811492	1.58	0.02630268	2.58E-05	2.95E-01	8.41E-07	1.53E-17	3.80189E-13	0.67195	0.279084	0.01	0.035832
13				1.089838	1.59	0.025703958	2.43E-05	3.00E-01	8.74E-07	1.63E-17	3.89045E-13	0.950665	0.278346	0.01	0.035927
14				1.367446	1.6	0.025118864	2.28E-05	3.05E-01	9.09E-07	1.74E-17	3.98107E-13	1.228642	0.277608	0.01	0.036022
15				1.644316	1.61	0.024547089	2.14E-05	3.09E-01	9.45E-07	1.85E-17	4.0738E-13	1.505881	0.276871	0.01	0.036118
16				1.920448	1.62	0.023988329	2.01E-05	3.14E-01	9.83E-07	1.97E-17	4.16869E-13	1.782382	0.276132	0.01	0.036215
17				2.19584	1.63	0.023442288	1.89E-05	3.19E-01	1.02E-06	2.09E-17	4.2658E-13	2.058144	0.275392	0.01	0.036312
18				2.470489	1.64	0.022908677	1.78E-05	3.24E-01	1.06E-06	2.23E-17	4.36516E-13	2.333165	0.274649	0.01	0.03641
19				2.744392	1.65	0.022387211	1.67E-05	3.29E-01	1.10E-06	2.37E-17	4.46684E-13	2.607441	0.273903	0.01	0.036509
20				3.017545	1.66	0.021877616	1.57E-05	3.35E-01	1.15E-06	2.52E-17	4.57088E-13	2.880969	0.273153	0.01	0.03661
21				3.289943	1.67	0.021379621	1.48E-05	3.40E-01	1.19E-06	2.68E-17	4.67735E-13	3.153744	0.272398	0.01	0.036711
22				3.56158	1.68	0.020892961	1.39E-05	3.45E-01	1.24E-06	2.84E-17	4.7863E-13	3.425762	0.271637	0.01	0.036814
23				3.83245	1.69	0.020417379	1.31E-05	3.50E-01	1.29E-06	3.02E-17	4.89779E-13	3.697015	0.270869	0.01	0.036918
24				4.102544	1.7	0.019952623	1.23E-05	3.55E-01	1.34E-06	3.21E-17	5.01187E-13	3.967497	0.270094	0.01	0.037024
25				4.371855	1.71	0.019498446	1.16E-05	3.61E-01	1.39E-06	3.42E-17	5.12861E-13	4.237199	0.269311	0.01	0.037132
26				4.640372	1.72	0.019054607	1.09E-05	3.66E-01	1.44E-06	3.63E-17	5.24807E-13	4.506113	0.268517	0.01	0.037242
27				4.908086	1.73	0.018620871	1.03E-05	3.71E-01	1.50E-06	3.86E-17	5.37032E-13	4.774229	0.267714	0.01	0.037353
28				5.174986	1.74	0.018197009	9.67E-06	3.77E-01	1.55E-06	4.10E-17	5.49541E-13	5.041536	0.2669	0.01	0.037467
29				5.441058	1.75	0.017782794	9.10E-06	3.82E-01	1.61E-06	4.35E-17	5.62341E-13	5.308022	0.266073	0.01	0.037584
30				5.706292	1.76	0.017378008	8.57E-06	3.88E-01	1.67E-06	4.62E-17	5.7544E-13	5.573675	0.265233	0.01	0.037703
31				5.970672	1.77	0.016982437	8.07E-06	3.93E-01	1.74E-06	4.91E-17	5.88844E-13	5.838482	0.26438	0.01	0.037824
32				6.234184	1.78	0.016595869	7.60E-06	3.99E-01	1.80E-06	5.21E-17	6.0256E-13	6.102428	0.263512	0.01	0.037949
33				6.496812	1.79	0.016218101	7.16E-06	4.04E-01	1.87E-06	5.53E-17	6.16595E-13	6.365498	0.262628	0.01	0.038077
34				6.75854	1.8	0.015848932	6.74E-06	4.10E-01	1.94E-06	5.87E-17	6.30957E-13	6.627676	0.261728	0.01	0.038208
35				7.019351	1.81	0.015488166	6.35E-06	4.15E-01	2.01E-06	6.23E-17	6.45654E-13	6.888946	0.260811	0.01	0.038342
36				7.279227	1.82	0.015135612	5.99E-06	4.21E-01	2.09E-06	6.61E-17	6.60693E-13	7.149289	0.259876	0.01	0.03848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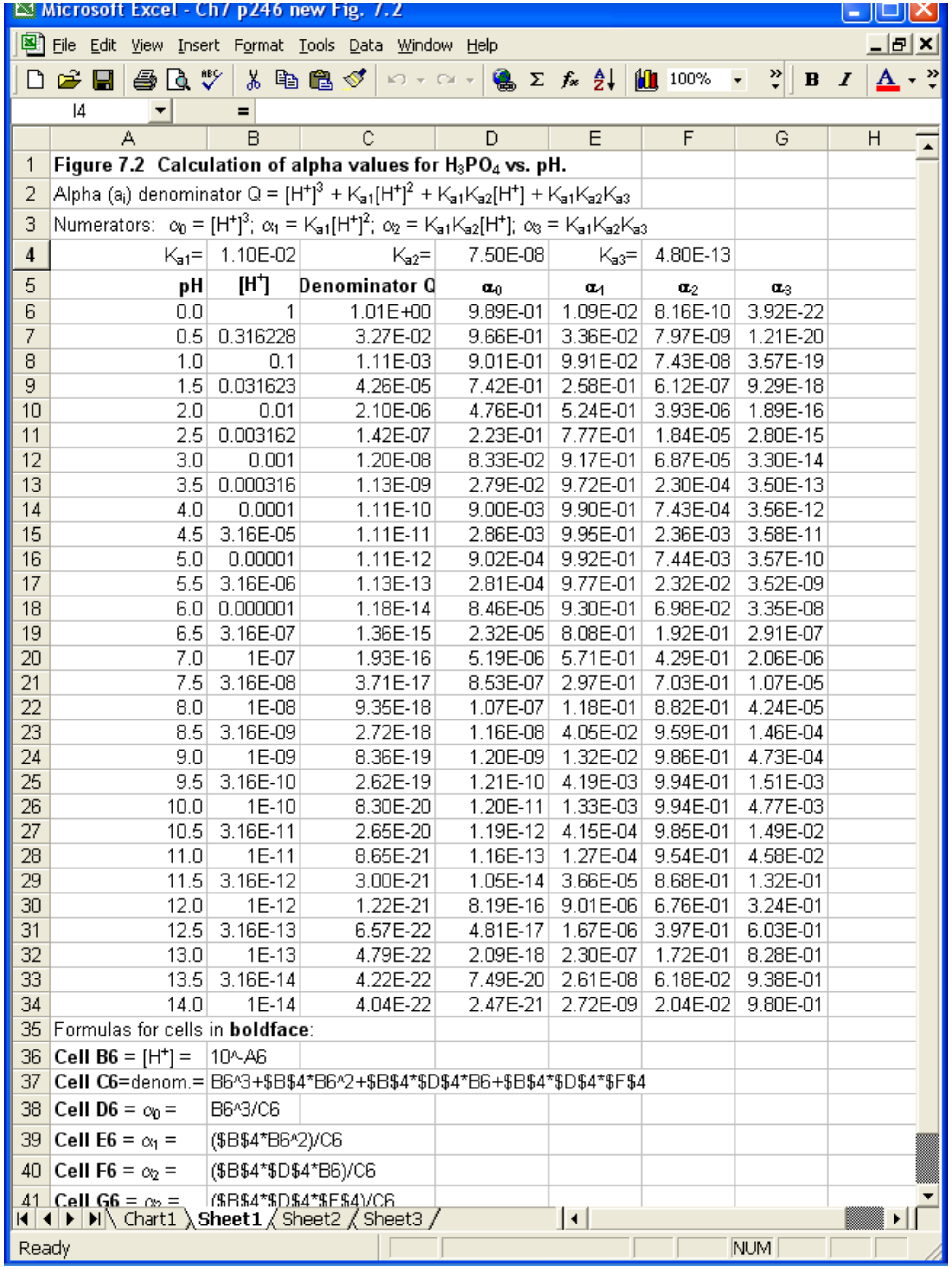
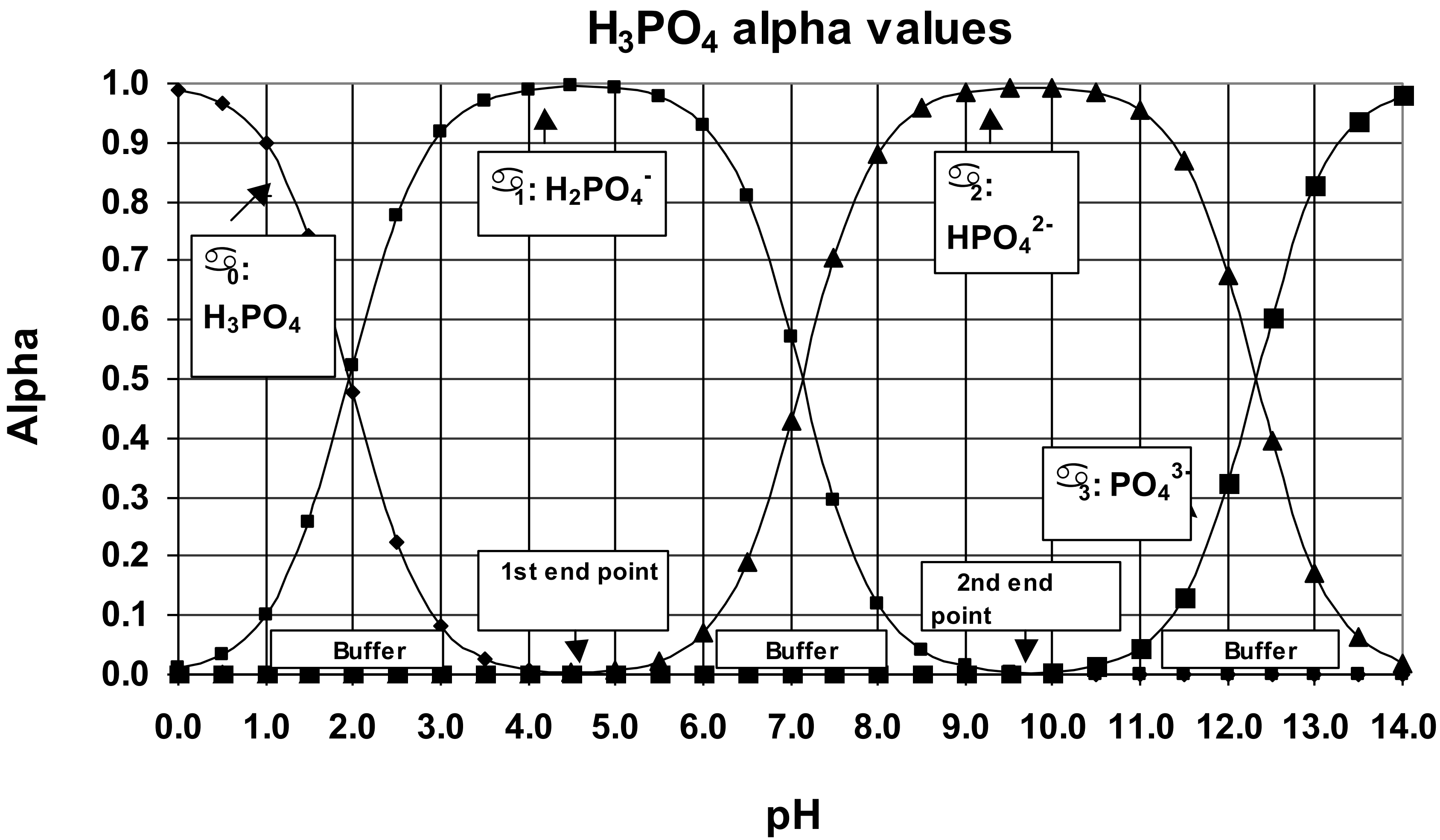
File Edit View Insert Format Tools Chart Window Help
97%
14
12
10
8
6
4
2
0
pH and First Derivative
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
Second Derivative
0
10
20
30
40
50
60
70
80
Volume Base Added, mL
1st derivative
pH vs VB
Plot Area
Beta vs pH
Buffer Intensity and Capacity
1st and 2nd deriv
Calculations
Ready
NUM

H_3PO_4 alpha vs. pH

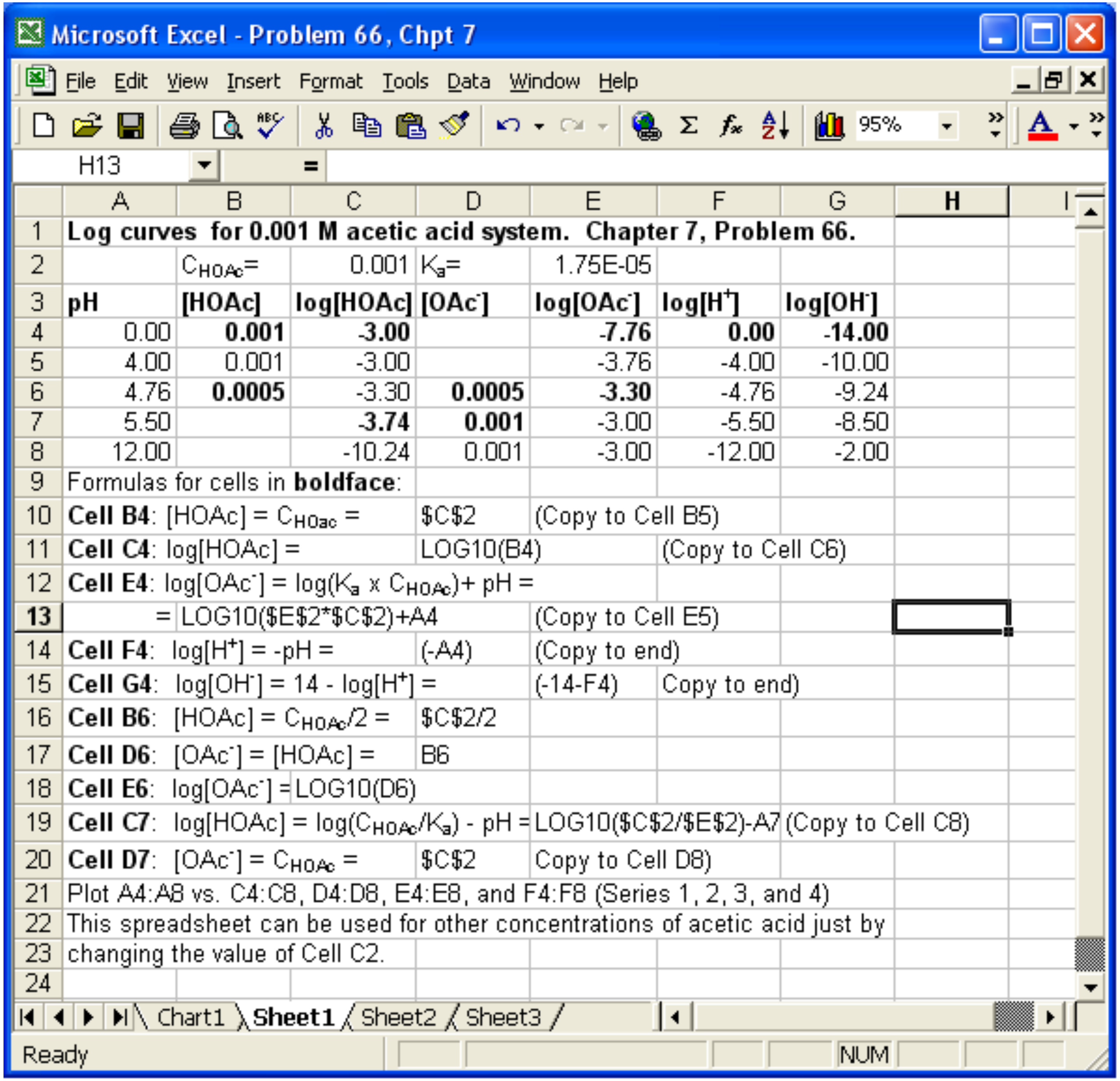


	A	B	C	D	E	F	G	H
1	**Figure 7.2 Calculation of alpha values for H_3PO_4 vs. pH.**							
2	Alpha (a_i) denominator Q = $[H^+]^3 + K_{a1}[H^+]^2 + K_{a1}K_{a2}[H^+] + K_{a1}K_{a2}K_{a3}$							
3	Numerators: $\alpha_0 = [H^+]^3$; $\alpha_1 = K_{a1}[H^+]^2$; $\alpha_2 = K_{a1}K_{a2}[H^+]$; $\alpha_3 = K_{a1}K_{a2}K_{a3}$							
4	K_{a1}=	1.10E-02	K_{a2}=	7.50E-08	K_{a3}=	4.80E-13		
5	**pH**	**$[H^+]$**	**Denominator Q**	**α_0**	**α_1**	**α_2**	**α_3**	
6	0.0	1	1.01E+00	9.89E-01	1.09E-02	8.16E-10	3.92E-22	
7	0.5	0.316228	3.27E-02	9.66E-01	3.36E-02	7.97E-09	1.21E-20	
8	1.0	0.1	1.11E-03	9.01E-01	9.91E-02	7.43E-08	3.57E-19	
9	1.5	0.031623	4.26E-05	7.42E-01	2.58E-01	6.12E-07	9.29E-18	
10	2.0	0.01	2.10E-06	4.76E-01	5.24E-01	3.93E-06	1.89E-16	
11	2.5	0.003162	1.42E-07	2.23E-01	7.77E-01	1.84E-05	2.80E-15	
12	3.0	0.001	1.20E-08	8.33E-02	9.17E-01	6.87E-05	3.30E-14	
13	3.5	0.000316	1.13E-09	2.79E-02	9.72E-01	2.30E-04	3.50E-13	
14	4.0	0.0001	1.11E-10	9.00E-03	9.90E-01	7.43E-04	3.56E-12	
15	4.5	3.16E-05	1.11E-11	2.86E-03	9.95E-01	2.36E-03	3.58E-11	
16	5.0	0.00001	1.11E-12	9.02E-04	9.92E-01	7.44E-03	3.57E-10	
17	5.5	3.16E-06	1.13E-13	2.81E-04	9.77E-01	2.32E-02	3.52E-09	
18	6.0	0.000001	1.18E-14	8.46E-05	9.30E-01	6.98E-02	3.35E-08	
19	6.5	3.16E-07	1.36E-15	2.32E-05	8.08E-01	1.92E-01	2.91E-07	
20	7.0	1E-07	1.93E-16	5.19E-06	5.71E-01	4.29E-01	2.06E-06	
21	7.5	3.16E-08	3.71E-17	8.53E-07	2.97E-01	7.03E-01	1.07E-05	
22	8.0	1E-08	9.35E-18	1.07E-07	1.18E-01	8.82E-01	4.24E-05	
23	8.5	3.16E-09	2.72E-18	1.16E-08	4.05E-02	9.59E-01	1.46E-04	
24	9.0	1E-09	8.36E-19	1.20E-09	1.32E-02	9.86E-01	4.73E-04	
25	9.5	3.16E-10	2.62E-19	1.21E-10	4.19E-03	9.94E-01	1.51E-03	
26	10.0	1E-10	8.30E-20	1.20E-11	1.33E-03	9.94E-01	4.77E-03	
27	10.5	3.16E-11	2.65E-20	1.19E-12	4.15E-04	9.85E-01	1.49E-02	
28	11.0	1E-11	8.65E-21	1.16E-13	1.27E-04	9.54E-01	4.58E-02	
29	11.5	3.16E-12	3.00E-21	1.05E-14	3.66E-05	8.68E-01	1.32E-01	
30	12.0	1E-12	1.22E-21	8.19E-16	9.01E-06	6.76E-01	3.24E-01	
31	12.5	3.16E-13	6.57E-22	4.81E-17	1.67E-06	3.97E-01	6.03E-01	
32	13.0	1E-13	4.79E-22	2.09E-18	2.30E-07	1.72E-01	8.28E-01	
33	13.5	3.16E-14	4.22E-22	7.49E-20	2.61E-08	6.18E-02	9.38E-01	
34	14.0	1E-14	4.04E-22	2.47E-21	2.72E-09	2.04E-02	9.80E-01	
35	Formulas for cells in **boldface**:							
36	**Cell B6** = $[H^+]$ =	10^A6						
37	**Cell C6**=denom.=	B6^3+$B$4*B6^2+$B$4*$D$4*B6+$B$4*$D$4*$F$4						
38	**Cell D6** = α_0 =	B6^3/C6						
39	**Cell E6** = α_1 =	($B$4*B6^2)/C6						
40	**Cell F6** = α_2 =	($B$4*$D$4*B6)/C6						
41	**Cell G6** = α_3 =	($B$4*$D$4*$F$4)/C6						

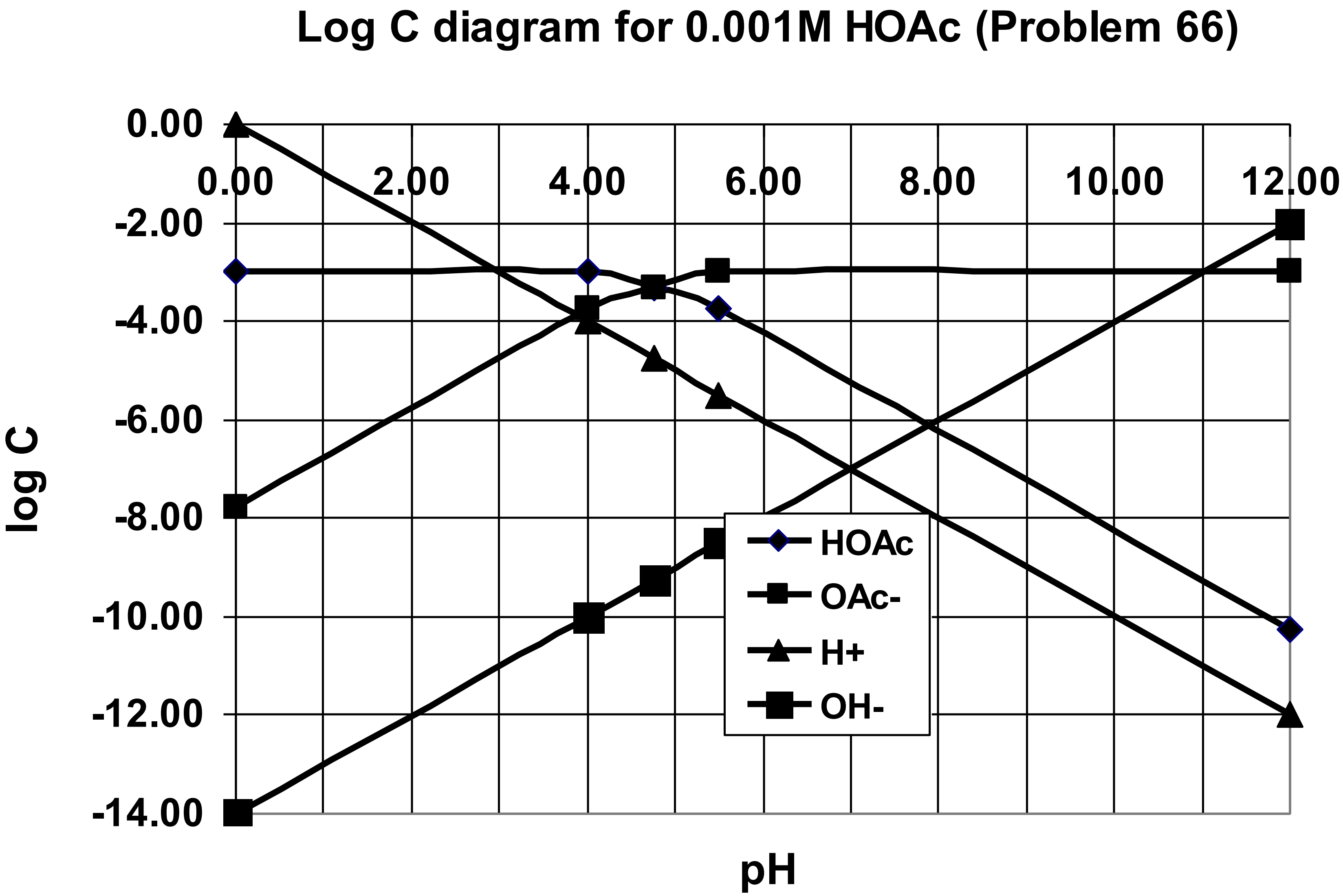


H₃PO₄ alpha values
Alpha
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
pH
♋0: H3PO4
♋1: H2PO4-
♋2: HPO42-
♋3: PO43-
1st end point
2nd end point
Buffer
Buffer
Buffer

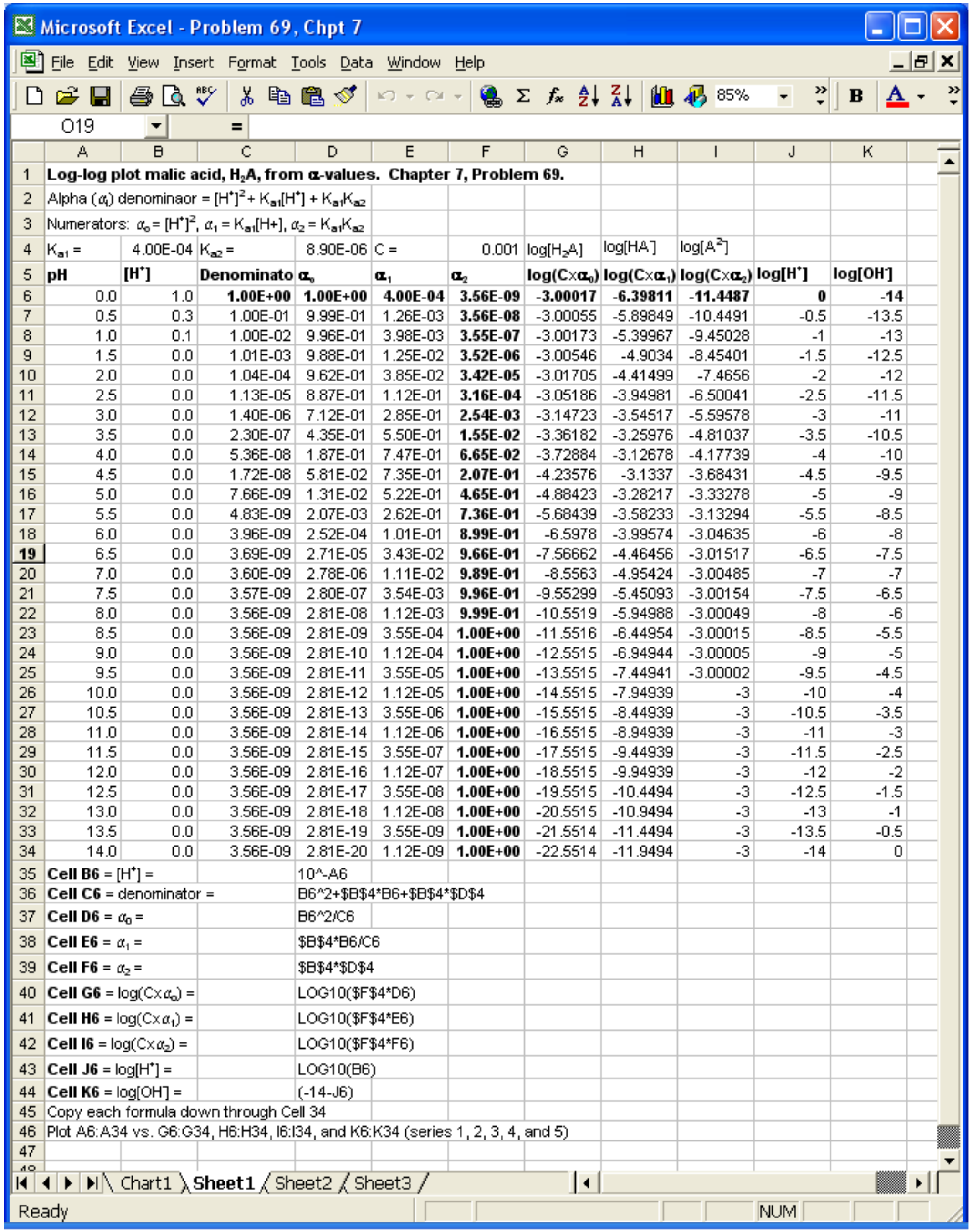
HOAc
logC vs. pH



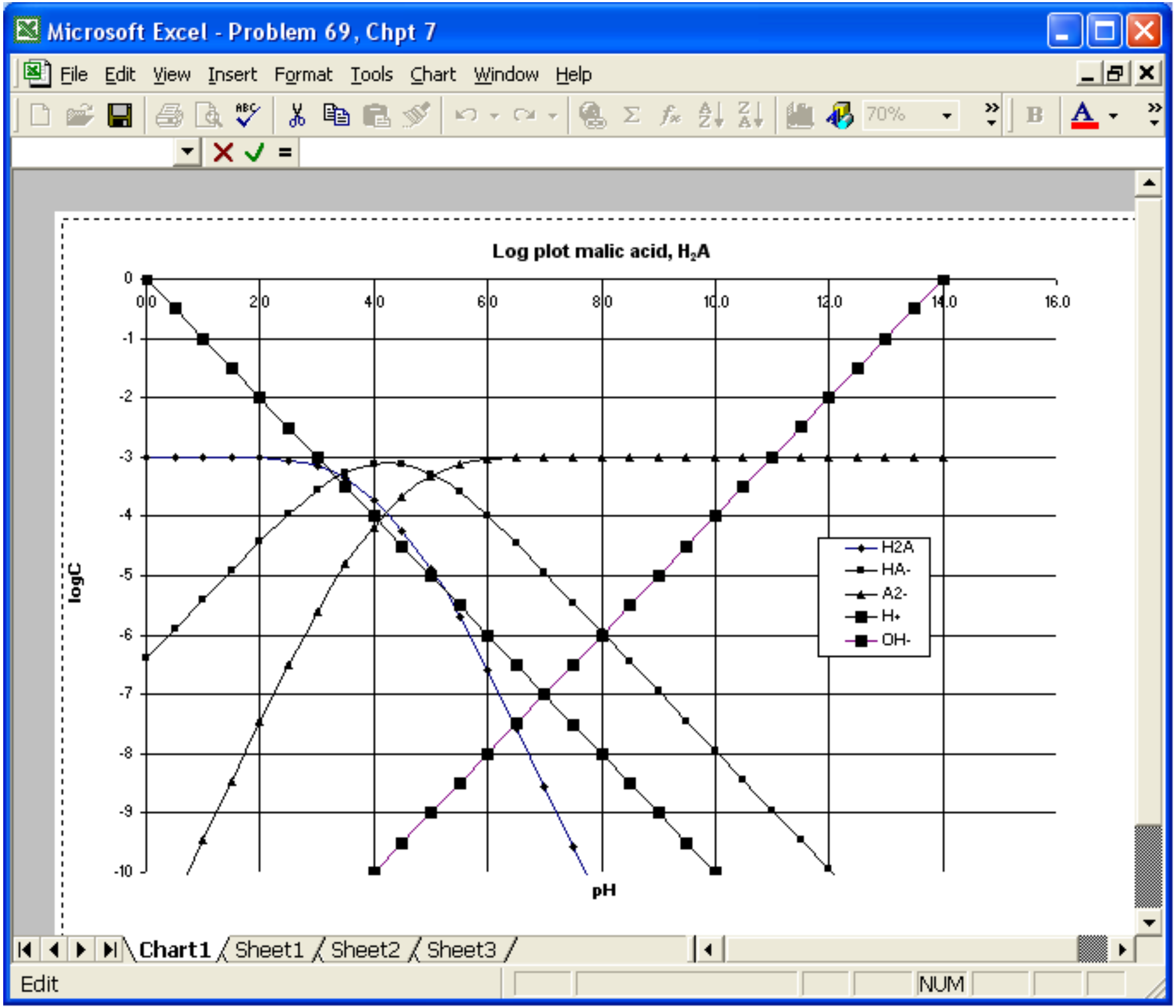
	A	B	C	D	E	F	G	H
1	**Log curves for 0.001 M acetic acid system. Chapter 7, Problem 66.**							
2		C_{HOAc}=	0.001	K_a=	1.75E-05			
3	**pH**	**[HOAc]**	**log[HOAc]**	**[OAc$^-$]**	**log[OAc$^-$]**	**log[H$^+$]**	**log[OH$^-$]**	
4	0.00	**0.001**	**-3.00**		**-7.76**	**0.00**	**-14.00**	
5	4.00	0.001	-3.00		-3.76	-4.00	-10.00	
6	4.76	**0.0005**	-3.30	**0.0005**	**-3.30**	-4.76	-9.24	
7	5.50		**-3.74**	**0.001**	-3.00	-5.50	-8.50	
8	12.00		-10.24	0.001	-3.00	-12.00	-2.00	
9	Formulas for cells in **boldface**:							
10	**Cell B4**: [HOAc] = C_{HOac} =			`$C$2`	(Copy to Cell B5)			
11	**Cell C4**: log[HOAc] =			LOG10(B4)		(Copy to Cell C6)		
12	**Cell E4**: log[OAc$^-$] = log(K_a x C_{HOAc})+ pH =							
13	=	`LOG10($E$2*$C$2)+A4`			(Copy to Cell E5)			
14	**Cell F4**: log[H$^+$] = -pH =			(-A4)	(Copy to end)			
15	**Cell G4**: log[OH$^-$] = 14 - log[H$^+$] =				(-14-F4)	Copy to end)		
16	**Cell B6**: [HOAc] = $C_{HOAc}/2$ =			`$C$2/2`				
17	**Cell D6**: [OAc$^-$] = [HOAc] =			B6				
18	**Cell E6**: log[OAc$^-$] =		LOG10(D6)					
19	**Cell C7**: log[HOAc] = log(C_{HOAc}/K_a) - pH =				`LOG10($C$2/$E$2)-A7`		(Copy to Cell C8)	
20	**Cell D7**: [OAc$^-$] = C_{HOAc} =			`$C$2`	Copy to Cell D8)			
21	Plot A4:A8 vs. C4:C8, D4:D8, E4:E8, and F4:F8 (Series 1, 2, 3, and 4)							
22	This spreadsheet can be used for other concentrations of acetic acid just by							
23	changing the value of Cell C2.							
24								


Log C diagram for 0.001M HOAc (Problem 66)
0.00
-2.00
-4.00
-6.00
-8.00
-10.00
-12.00
-14.00
0.00
2.00
4.00
6.00
8.00
10.00
12.00
log C
pH
HOAc
OAc-
H+
OH-

H_2A, malic acid
logC vs. pH



	A	B	C	D	E	F	G	H	I	J	K
1	**Log-log plot malic acid, H_2A, from α-values. Chapter 7, Problem 69.**										
2	Alpha (α_i) denominaor = $[H^+]^2 + K_{a1}[H^+] + K_{a1}K_{a2}$										
3	Numerators: $\alpha_o = [H^+]^2$, $\alpha_1 = K_{a1}[H+]$, $\alpha_2 = K_{a1}K_{a2}$										
4	K_{a1} =	4.00E-04	K_{a2} =	8.90E-06	C =	0.001	$\log[H_2A]$	$\log[HA^-]$	$\log[A^{2-}]$		
5	**pH**	**$[H^+]$**	**Denominato**	**α_o**	**α_1**	**α_2**	**$\log(C\times\alpha_0)$**	**$\log(C\times\alpha_1)$**	**$\log(C\times\alpha_2)$**	**$\log[H^+]$**	**$\log[OH^-]$**
6	0.0	1.0	**1.00E+00**	**1.00E+00**	**4.00E-04**	**3.56E-09**	**-3.00017**	**-6.39811**	**-11.4487**	**0**	**-14**
7	0.5	0.3	1.00E-01	9.99E-01	1.26E-03	**3.56E-08**	-3.00055	-5.89849	-10.4491	-0.5	-13.5
8	1.0	0.1	1.00E-02	9.96E-01	3.98E-03	**3.55E-07**	-3.00173	-5.39967	-9.45028	-1	-13
9	1.5	0.0	1.01E-03	9.88E-01	1.25E-02	**3.52E-06**	-3.00546	-4.9034	-8.45401	-1.5	-12.5
10	2.0	0.0	1.04E-04	9.62E-01	3.85E-02	**3.42E-05**	-3.01705	-4.41499	-7.4656	-2	-12
11	2.5	0.0	1.13E-05	8.87E-01	1.12E-01	**3.16E-04**	-3.05186	-3.94981	-6.50041	-2.5	-11.5
12	3.0	0.0	1.40E-06	7.12E-01	2.85E-01	**2.54E-03**	-3.14723	-3.54517	-5.59578	-3	-11
13	3.5	0.0	2.30E-07	4.35E-01	5.50E-01	**1.55E-02**	-3.36182	-3.25976	-4.81037	-3.5	-10.5
14	4.0	0.0	5.36E-08	1.87E-01	7.47E-01	**6.65E-02**	-3.72884	-3.12678	-4.17739	-4	-10
15	4.5	0.0	1.72E-08	5.81E-02	7.35E-01	**2.07E-01**	-4.23576	-3.1337	-3.68431	-4.5	-9.5
16	5.0	0.0	7.66E-09	1.31E-02	5.22E-01	**4.65E-01**	-4.88423	-3.28217	-3.33278	-5	-9
17	5.5	0.0	4.83E-09	2.07E-03	2.62E-01	**7.36E-01**	-5.68439	-3.58233	-3.13294	-5.5	-8.5
18	6.0	0.0	3.96E-09	2.52E-04	1.01E-01	**8.99E-01**	-6.5978	-3.99574	-3.04635	-6	-8
19	6.5	0.0	3.69E-09	2.71E-05	3.43E-02	**9.66E-01**	-7.56662	-4.46456	-3.01517	-6.5	-7.5
20	7.0	0.0	3.60E-09	2.78E-06	1.11E-02	**9.89E-01**	-8.5563	-4.95424	-3.00485	-7	-7
21	7.5	0.0	3.57E-09	2.80E-07	3.54E-03	**9.96E-01**	-9.55299	-5.45093	-3.00154	-7.5	-6.5
22	8.0	0.0	3.56E-09	2.81E-08	1.12E-03	**9.99E-01**	-10.5519	-5.94988	-3.00049	-8	-6
23	8.5	0.0	3.56E-09	2.81E-09	3.55E-04	**1.00E+00**	-11.5516	-6.44954	-3.00015	-8.5	-5.5
24	9.0	0.0	3.56E-09	2.81E-10	1.12E-04	**1.00E+00**	-12.5515	-6.94944	-3.00005	-9	-5
25	9.5	0.0	3.56E-09	2.81E-11	3.55E-05	**1.00E+00**	-13.5515	-7.44941	-3.00002	-9.5	-4.5
26	10.0	0.0	3.56E-09	2.81E-12	1.12E-05	**1.00E+00**	-14.5515	-7.94939	-3	-10	-4
27	10.5	0.0	3.56E-09	2.81E-13	3.55E-06	**1.00E+00**	-15.5515	-8.44939	-3	-10.5	-3.5
28	11.0	0.0	3.56E-09	2.81E-14	1.12E-06	**1.00E+00**	-16.5515	-8.94939	-3	-11	-3
29	11.5	0.0	3.56E-09	2.81E-15	3.55E-07	**1.00E+00**	-17.5515	-9.44939	-3	-11.5	-2.5
30	12.0	0.0	3.56E-09	2.81E-16	1.12E-07	**1.00E+00**	-18.5515	-9.94939	-3	-12	-2
31	12.5	0.0	3.56E-09	2.81E-17	3.55E-08	**1.00E+00**	-19.5515	-10.4494	-3	-12.5	-1.5
32	13.0	0.0	3.56E-09	2.81E-18	1.12E-08	**1.00E+00**	-20.5515	-10.9494	-3	-13	-1
33	13.5	0.0	3.56E-09	2.81E-19	3.55E-09	**1.00E+00**	-21.5514	-11.4494	-3	-13.5	-0.5
34	14.0	0.0	3.56E-09	2.81E-20	1.12E-09	**1.00E+00**	-22.5514	-11.9494	-3	-14	0
35	**Cell B6** = $[H^+]$ =			`10^-A6`							
36	**Cell C6** = denominator =			`B6^2+$B$4*B6+$B$4*$D$4`							
37	**Cell D6** = α_0 =			`B6^2/C6`							
38	**Cell E6** = α_1 =			`$B$4*B6/C6`							
39	**Cell F6** = α_2 =			`$B$4*$D$4`							
40	**Cell G6** = $\log(C\times\alpha_o)$ =			`LOG10($F$4*D6)`							
41	**Cell H6** = $\log(C\times\alpha_1)$ =			`LOG10($F$4*E6)`							
42	**Cell I6** = $\log(C\times\alpha_2)$ =			`LOG10($F$4*F6)`							
43	**Cell J6** = $\log[H^+]$ =			`LOG10(B6)`							
44	**Cell K6** = log[OH] =			`(-14-J6)`							
45	Copy each formula down through Cell 34										
46	Plot A6:A34 vs. G6:G34, H6:H34, I6:I34, and K6:K34 (series 1, 2, 3, 4, and 5)										
47											


Microsoft Excel - Problem 69, Chpt 7
File
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70%
Log plot malic acid, H$_2$A
0
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
logC
pH
H2A
HA-
A2-
H+
OH-
Chart1
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Sheet2
Sheet3
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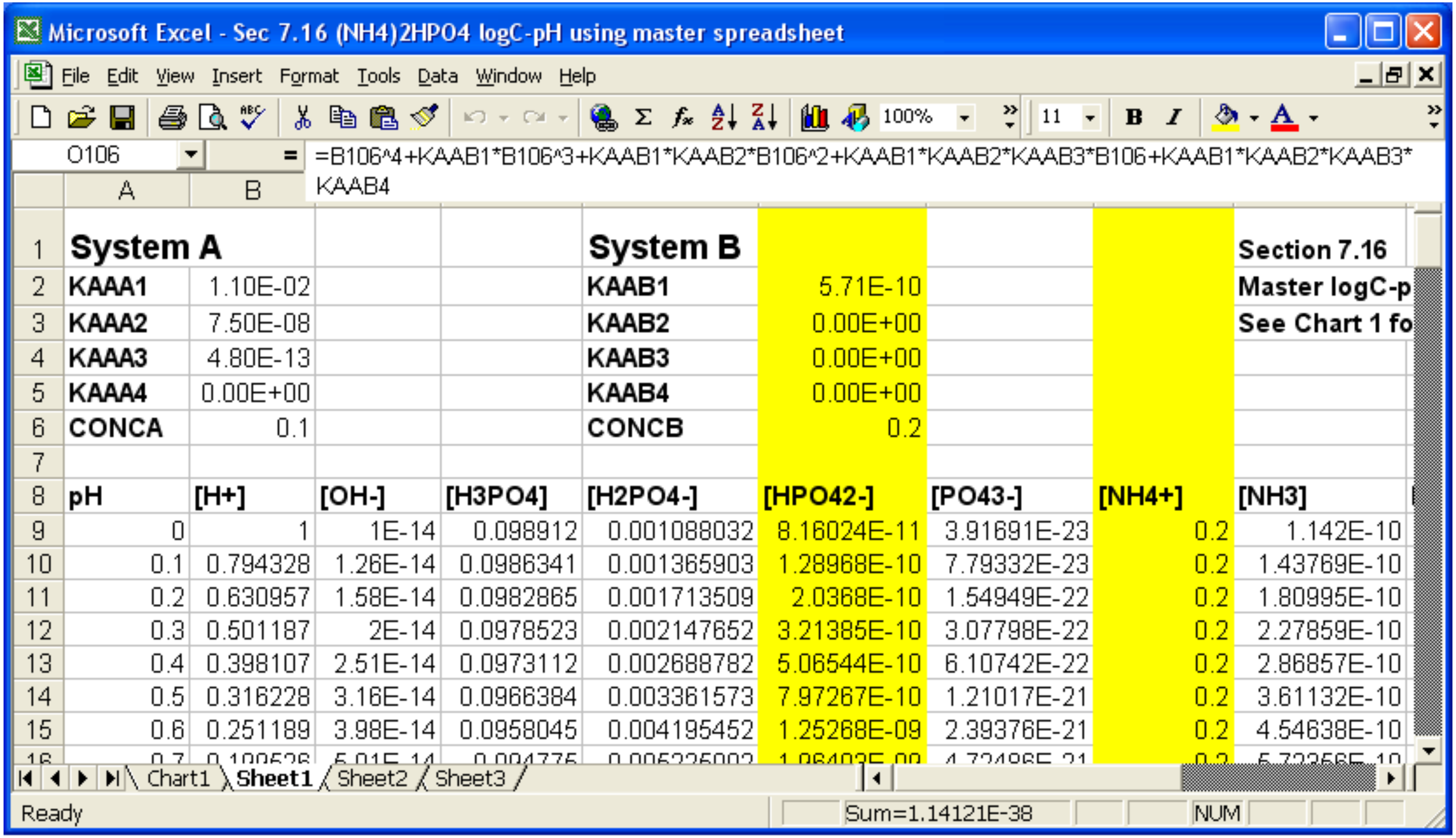
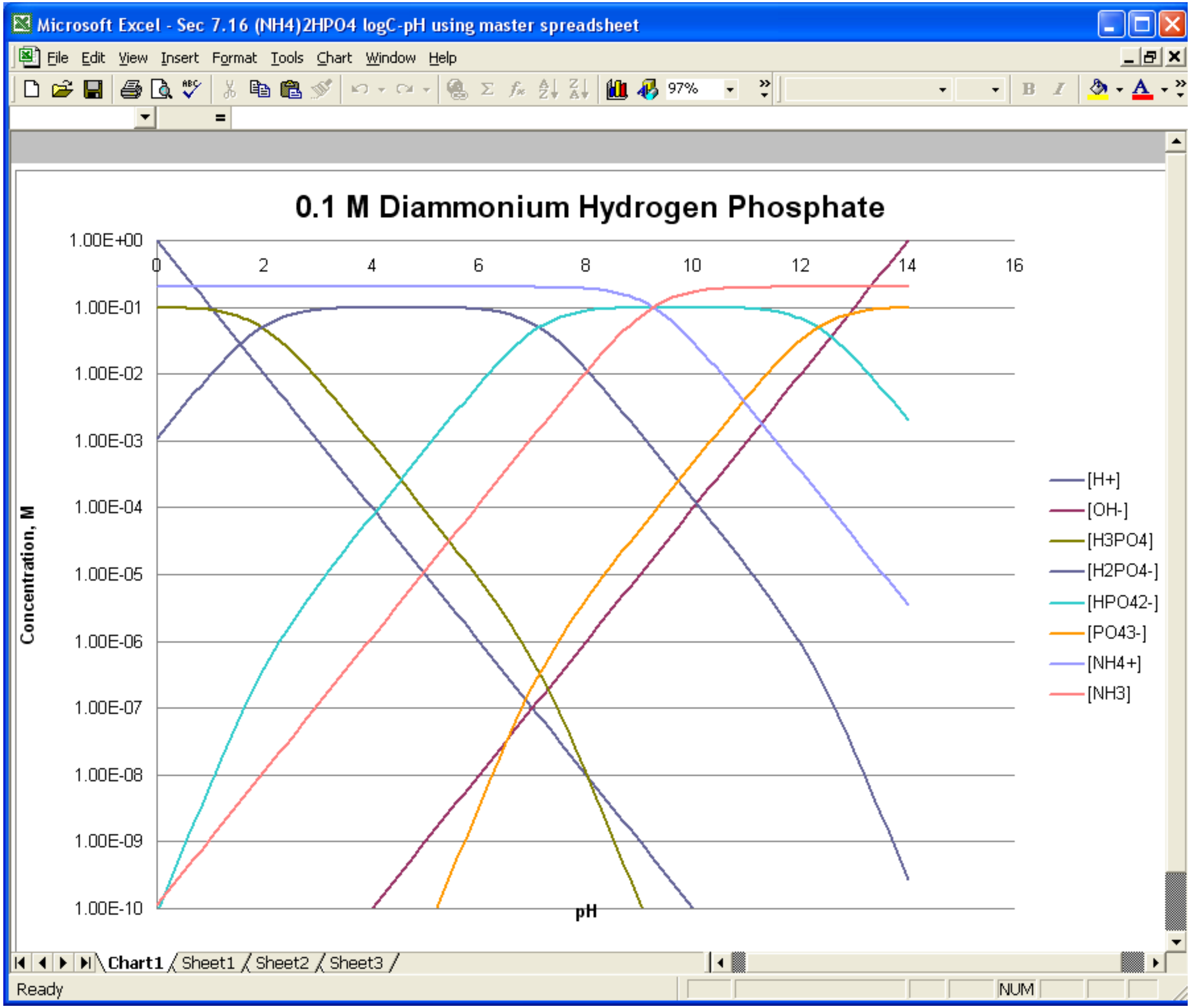
$(NH_4)_2HPO_4$ logC vs. pH plot



O106 = =B106^4+KAAB1*B106^3+KAAB1*KAAB2*B106^2+KAAB1*KAAB2*KAAB3*B106+KAAB1*KAAB2*KAAB3*KAAB4

	A	B							
1	**System A**				**System B**				**Section 7.16**
2	**KAAA1**	1.10E-02			**KAAB1**	5.71E-10			**Master logC-p**
3	**KAAA2**	7.50E-08			**KAAB2**	0.00E+00			**See Chart 1 fo**
4	**KAAA3**	4.80E-13			**KAAB3**	0.00E+00			
5	**KAAA4**	0.00E+00			**KAAB4**	0.00E+00			
6	**CONCA**	0.1			**CONCB**	0.2			
7									
8	**pH**	**[H+]**	**[OH-]**	**[H3PO4]**	**[H2PO4-]**	**[HPO42-]**	**[PO43-]**	**[NH4+]**	**[NH3]**
9	0	1	1E-14	0.098912	0.001088032	8.16024E-11	3.91691E-23	0.2	1.142E-10
10	0.1	0.794328	1.26E-14	0.0986341	0.001365903	1.28968E-10	7.79332E-23	0.2	1.43769E-10
11	0.2	0.630957	1.58E-14	0.0982865	0.001713509	2.0368E-10	1.54949E-22	0.2	1.80995E-10
12	0.3	0.501187	2E-14	0.0978523	0.002147652	3.21385E-10	3.07798E-22	0.2	2.27859E-10
13	0.4	0.398107	2.51E-14	0.0973112	0.002688782	5.06544E-10	6.10742E-22	0.2	2.86857E-10
14	0.5	0.316228	3.16E-14	0.0966384	0.003361573	7.97267E-10	1.21017E-21	0.2	3.61132E-10
15	0.6	0.251189	3.98E-14	0.0958045	0.004195452	1.25268E-09	2.39376E-21	0.2	4.54638E-10


Microsoft Excel - Sec 7.16 (NH4)2HPO4 logC-pH using master spreadsheet
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97%
0.1 M Diammonium Hydrogen Phosphate
Concentration, M
1.00E+00
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
1.00E-09
1.00E-10
0
2
4
6
8
10
12
14
16
pH
[H+]
[OH-]
[H3PO4]
[H2PO4-]
[HPO42-]
[PO43-]
[NH4+]
[NH3]
Chart1
Sheet1
Sheet2
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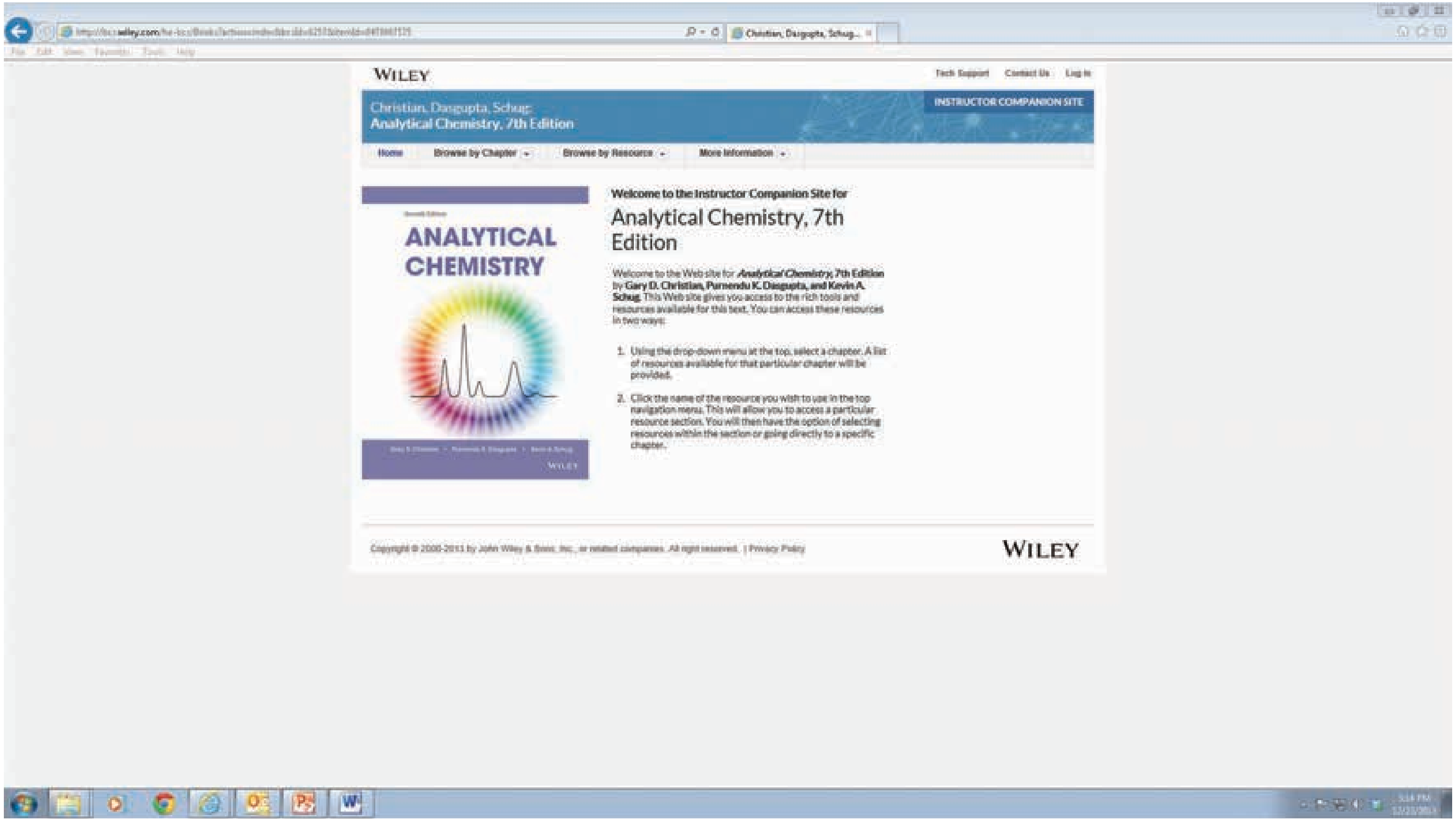

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1. Using the drop-down menu at the top, select a chapter. A list of resources available for that particular chapter will be provided.
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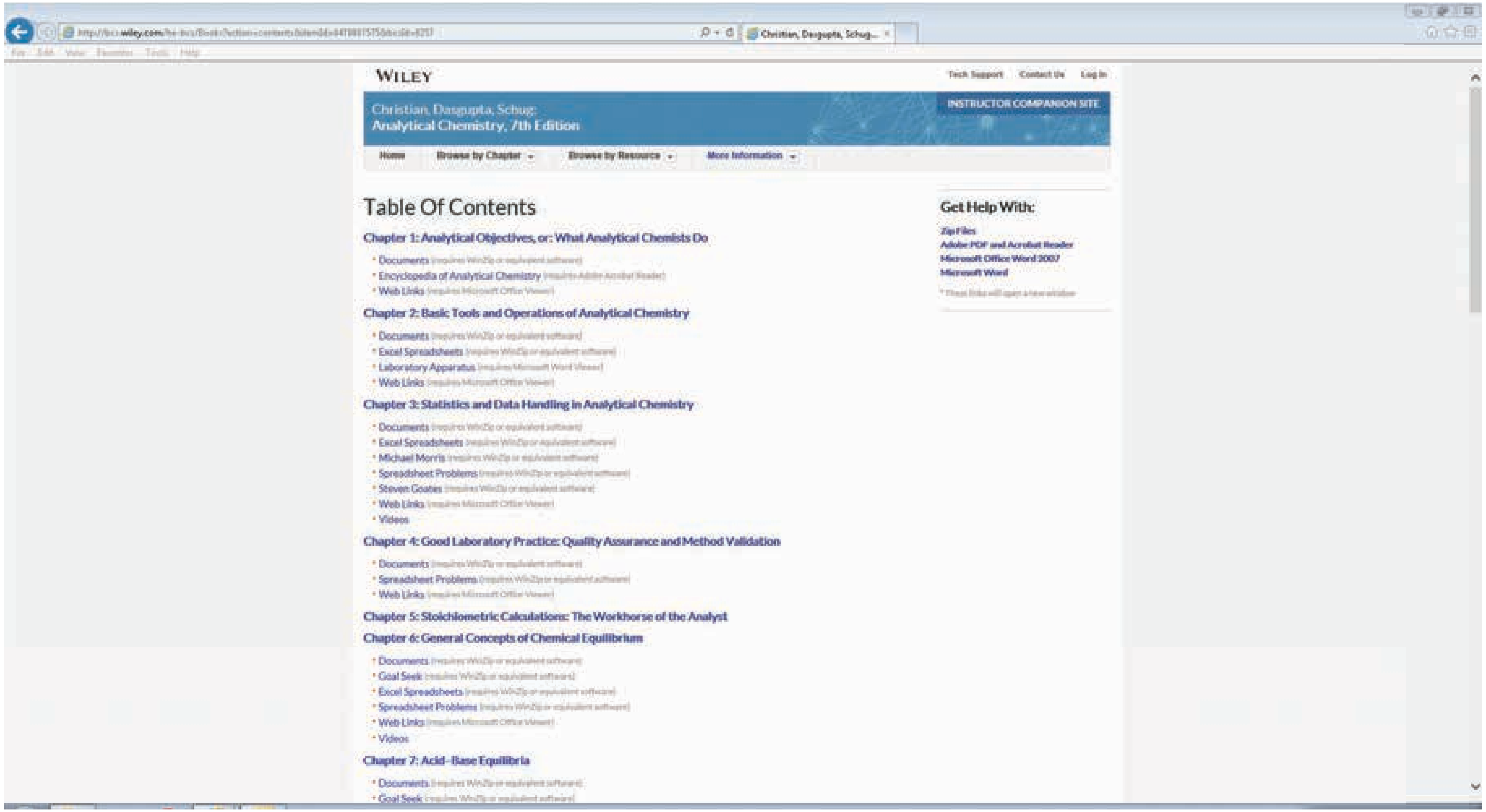

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Table Of Contents

Chapter 1: Analytical Objectives, or: What Analytical Chemists Do

- Documents (requires WinZip or equivalent software)
- Encyclopedia of Analytical Chemistry (requires Adobe Acrobat Reader)
- Web Links (requires Microsoft Office Viewer)

Chapter 2: Basic Tools and Operations of Analytical Chemistry

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- Excel Spreadsheets (requires WinZip or equivalent software)
- Laboratory Apparatus (requires Microsoft Word Viewer)
- Web Links (requires Microsoft Office Viewer)

Chapter 3: Statistics and Data Handling in Analytical Chemistry

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- Excel Spreadsheets (requires WinZip or equivalent software)
- Michael Morris (requires WinZip or equivalent software)
- Spreadsheet Problems (requires WinZip or equivalent software)
- Steven Goates (requires WinZip or equivalent software)
- Web Links (requires Microsoft Office Viewer)
- Videos

Chapter 4: Good Laboratory Practice: Quality Assurance and Method Validation

- Documents (requires WinZip or equivalent software)
- Spreadsheet Problems (requires WinZip or equivalent software)
- Web Links (requires Microsoft Office Viewer)

Chapter 5: Stoichiometric Calculations: The Workhorse of the Analyst

Chapter 6: General Concepts of Chemical Equilibrium

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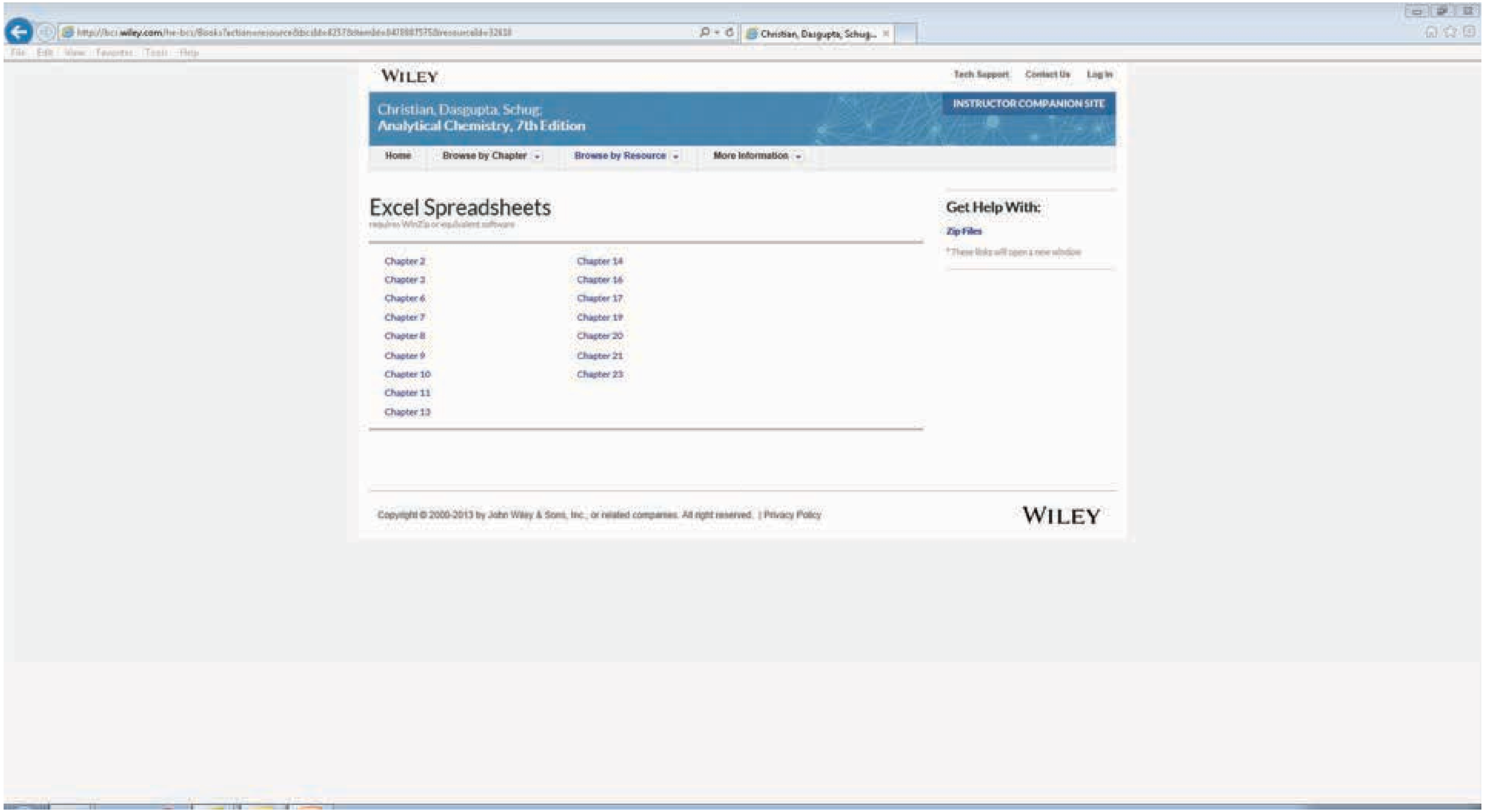

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- Chapter 2
- Chapter 3
- Chapter 6
- Chapter 7
- Chapter 8
- Chapter 9
- Chapter 10
- Chapter 11
- Chapter 13
- Chapter 14
- Chapter 16
- Chapter 17
- Chapter 19
- Chapter 20
- Chapter 21
- Chapter 23

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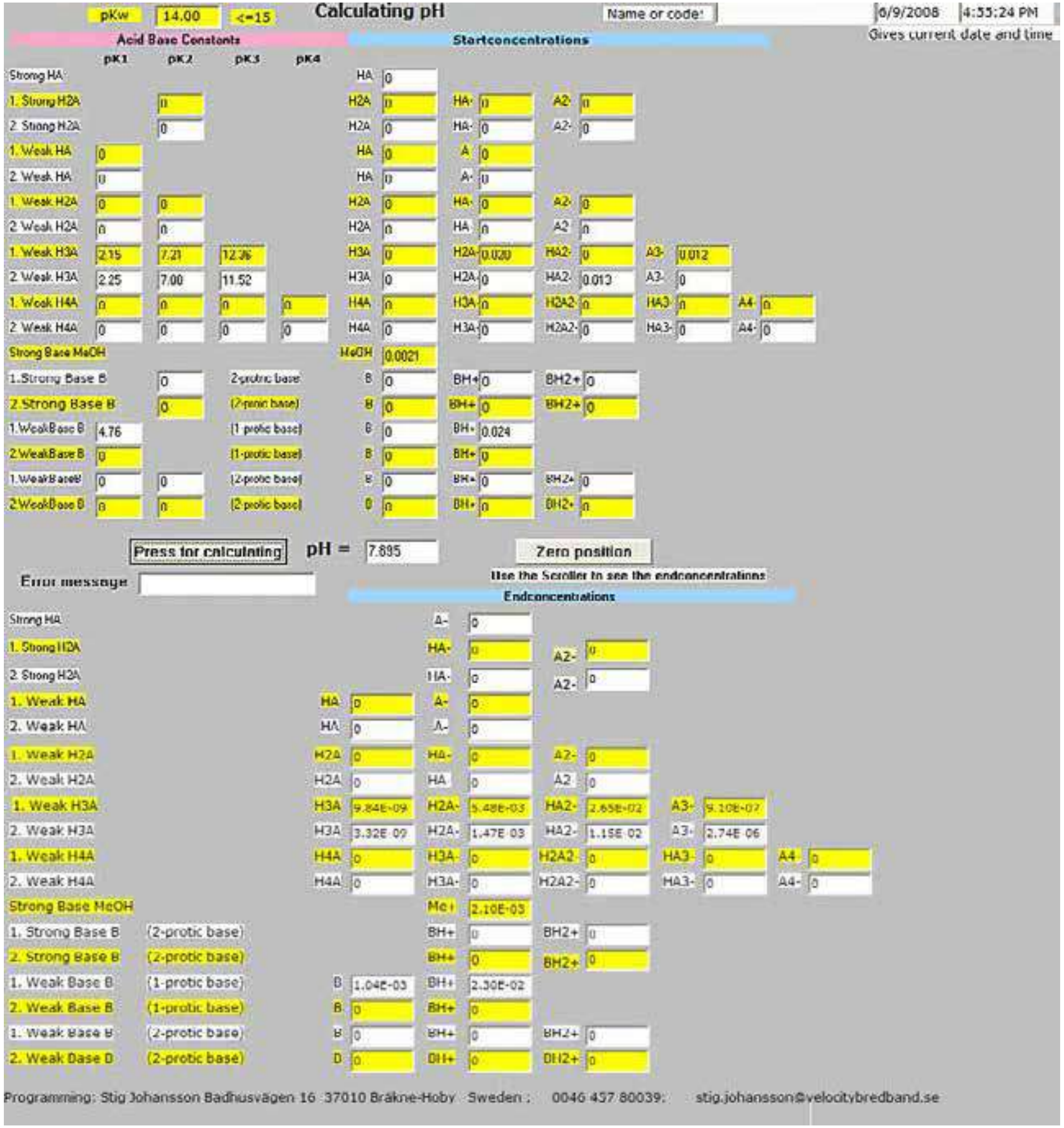
Calculate pH for a mixture of 0.012M $(NH_4)_2LiPO_4$, 0.020M NaH_2PO_4, 0.013M K_2HAsO_4 and 0.0021M NaOH.

H_3PO_4: pK1 =2.15 pK2 =7.21 pK3 =12.36
H_3A=0 H_2A^-=0.020 HA^{2-}=0 A^{3-}=0.012

H_3AsO_4: pK1=2.25 pK2 =7.00 pK3 =11.52
H_3A=0 H_2A^-=0 HA^{2-}=0.013 A^{3-}= 0

MeOH =0.0021

NH_4^+: Kb= 4.76
B = 0 BH^+ = 0.024



pKw 14.00 <=15

Calculating pH

Name or code:

6/9/2008 4:55:24 PM

Gives current date and time

Acid Base Constants	pK1	pK2	pK3	pK4	Startconcentrations									
Strong HA					HA	0								
1. Strong H2A		0			H2A	0	HA-	0	A2-	0				
2. Strong H2A		0			H2A	0	HA-	0	A2-	0				
1. Weak HA	0				HA	0	A	0						
2. Weak HA	0				HA	0	A-	0						
1. Weak H2A	0	0			H2A	0	HA-	0	A2-	0				
2. Weak H2A	0	0			H2A	0	HA	0	A2	0				
1. Weak H3A	2.15	7.21	12.36		H3A	0	H2A-	0.020	HA2-	0	A3-	0.012		
2. Weak H3A	2.25	7.00	11.52		H3A	0	H2A-	0	HA2-	0.013	A3-	0		
1. Weak H4A	0	0	0	0	H4A	0	H3A-	0	H2A2-	0	HA3-	0	A4-	0
2. Weak H4A	0	0	0	0	H4A	0	H3A-	0	H2A2-	0	HA3-	0	A4-	0
Strong Base MeOH					MeOH	0.0021								
1.Strong Base B		0	2-protic base		B	0	BH+	0	BH2+	0				
2.Strong Base B		0	(2-protic base)		B	0	BH+	0	BH2+	0				
1.WeakBase B	4.76		(1 protic base)		B	0	BH+	0.024						
2.WeakBase B	0		(1-protic base)		B	0	BH+	0						
1.WeakBaseB	0	0	(2-protic base)		B	0	BH+	0	BH2+	0				
2.WeakBase B	0	0	(2-protic base)		B	0	BH+	0	BH2+	0				

pH = 7.895

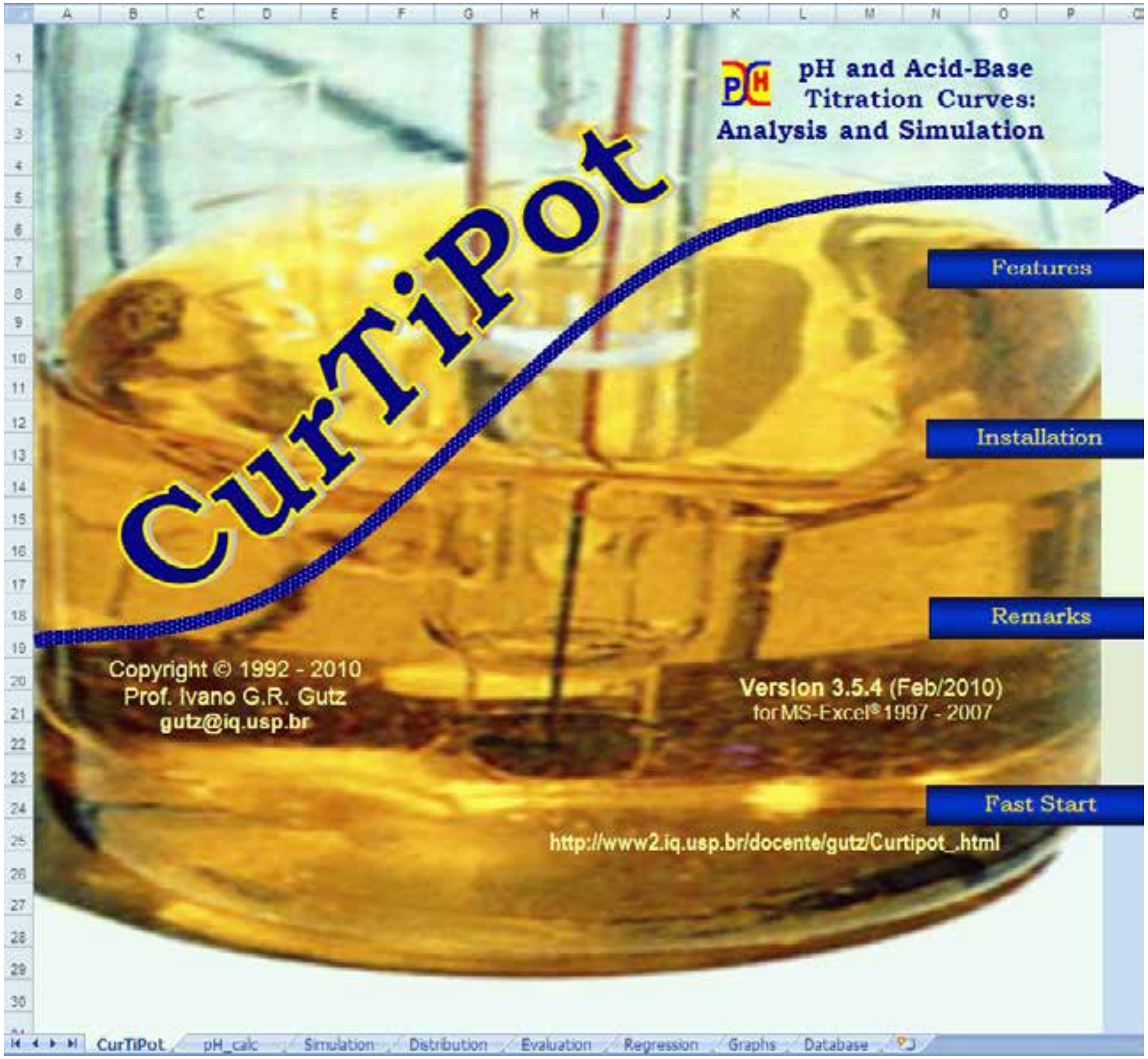
Error message

Use the Scroller to see the endconcentrations

		Endconcentrations									
Strong HA				A-	0						
1. Strong H2A				HA-	0	A2-	0				
2. Strong H2A				HA-	0	A2-	0				
1. Weak HA		HA	0	A-	0						
2. Weak HA		HA	0	A-	0						
1. Weak H2A		H2A	0	HA-	0	A2-	0				
2. Weak H2A		H2A	0	HA	0	A2	0				
1. Weak H3A		H3A	9.84E-09	H2A-	5.48E-03	HA2-	2.65E-02	A3-	9.10E-07		
2. Weak H3A		H3A	3.32E-09	H2A-	1.47E-03	HA2-	1.15E-02	A3-	2.74E-06		
1. Weak H4A		H4A	0	H3A-	0	H2A2-	0	HA3-	0	A4-	0
2. Weak H4A		H4A	0	H3A-	0	H2A2-	0	HA3-	0	A4-	0
Strong Base MeOH				Me+	2.10E-03						
1. Strong Base B	(2-protic base)			BH+	0	BH2+	0				
2. Strong Base B	(2-protic base)			BH+	0	BH2+	0				
1. Weak Base B	(1-protic base)	B	1.04E-03	BH+	2.30E-02						
2. Weak Base B	(1-protic base)	B	0	BH+	0						
1. Weak Base B	(2-protic base)	B	0	BH+	0	BH2+	0				
2. Weak Base B	(2-protic base)	B	0	BH+	0	BH2+	0				

Programming: Stig Johansson Badhusvägen 16 37010 Bräkne-Hoby Sweden ; 0046 457 80039; stig.johansson@velocitybredband.se

A very useful program is CurTiPot by Ivano Gutz, Universidad de São Paulo, Brazil:
http://www2.iq.usp.br/docente/gutz/Curtipot_.html



CurTiPot

pH and Acid-Base
Titration Curves:
Analysis and Simulation

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Prof. Ivano G.R. Gutz
gutz@iq.usp.br

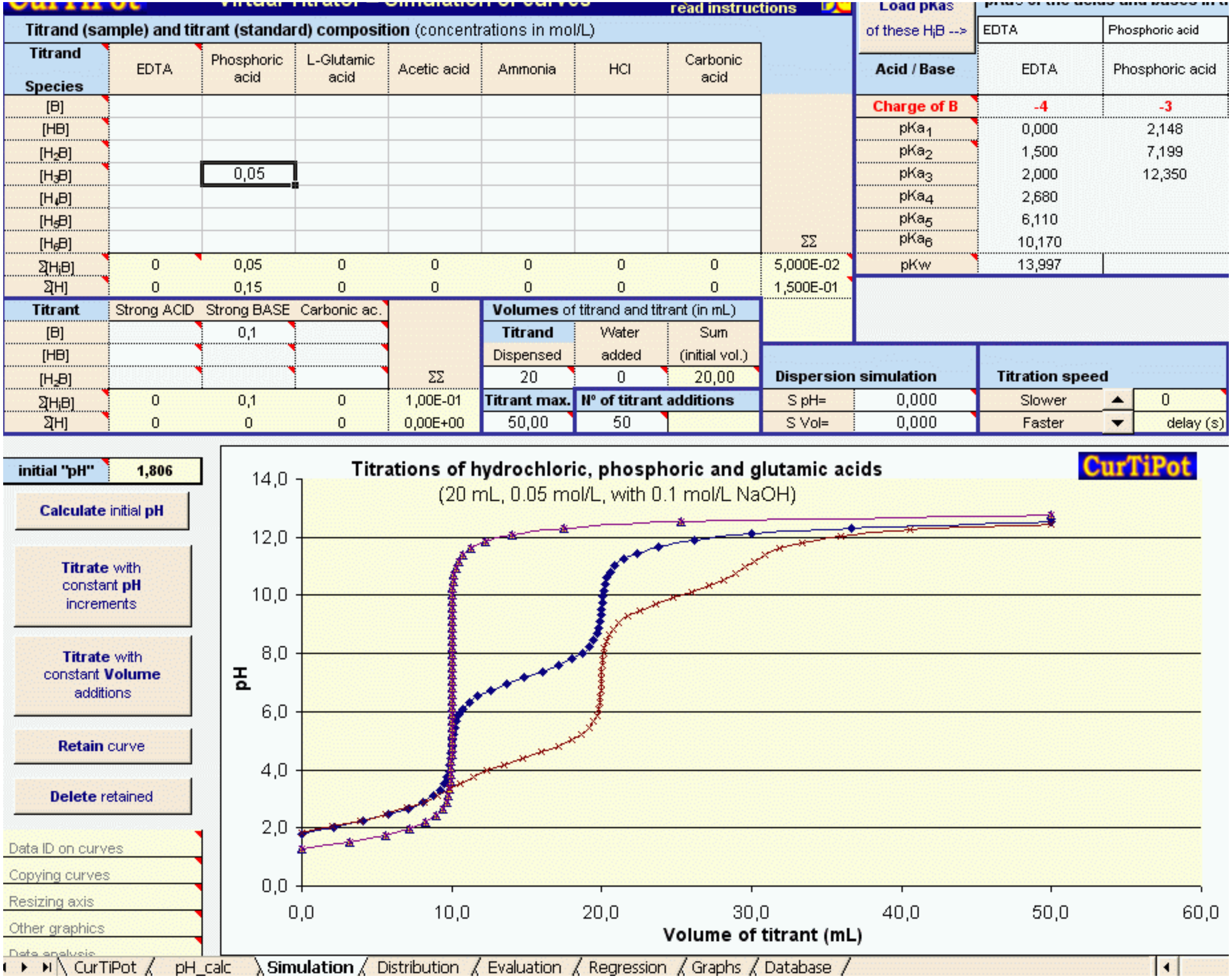
Version 3.5.4 (Feb/2010)
for MS-Excel® 1997 - 2007

http://www2.iq.usp.br/docente/gutz/Curtipot_.html

It is a powerful and very versatile program that performs pH and paH calculations, and also titration curves, alpha plots, etc.   It provides:

- pH calculation of any aqueous solution of acids, bases and salts, including buffers, zwitterionic amino acids, from single component to complex mixtures (30 or more species in equilibrium)

- Buffer capacity (buffer index, buffer strength), ionic strength, fractional distribution, medium charge of H_iB – to find the Isoelectric Point of amino acids –, activities and apparent dissociation constants of all species at equilibrium.



Titrand (sample) and titrant (standard) composition (concentrations in mol/L)

Titrand Species	EDTA	Phosphoric acid	L-Glutamic acid	Acetic acid	Ammonia	HCl	Carbonic acid	
[B]								
[HB]								
$[H_2B]$								
$[H_3B]$		0,05						
$[H_4B]$								
$[H_5B]$								
$[H_6B]$								ΣΣ
$\Sigma[H_iB]$	0	0,05	0	0	0	0	0	5,000E-02
Σ[H]	0	0,15	0	0	0	0	0	1,500E-01

	EDTA	Phosphoric acid
Acid / Base	EDTA	Phosphoric acid
Charge of B	**-4**	**-3**
pKa_1	0,000	2,148
pKa_2	1,500	7,199
pKa_3	2,000	12,350
pKa_4	2,680	
pKa_5	6,110	
pKa_6	10,170	
pKw	13,997	

Titrant	Strong ACID	Strong BASE	Carbonic ac.	
[B]		0,1		
[HB]				
$[H_2B]$				ΣΣ
$\Sigma[H_iB]$	0	0,1	0	1,00E-01
Σ[H]	0	0	0	0,00E+00

Volumes of titrand and titrant (in mL)

Titrand Dispensed	Water added	Sum (initial vol.)
20	0	20,00
Titrant max.	**Nº of titrant additions**	
50,00	50	

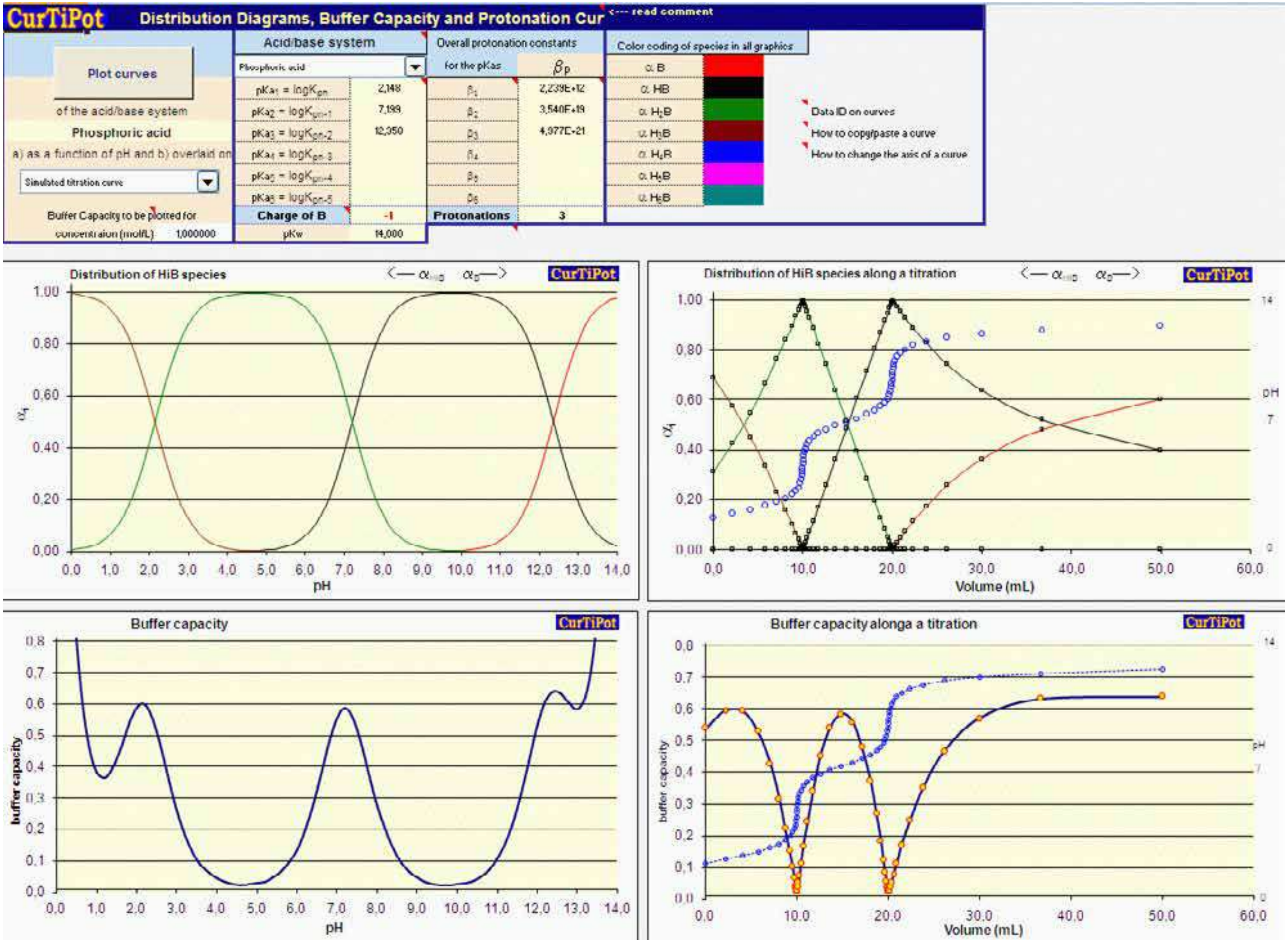
Dispersion simulation

S pH=	0,000
S Vol=	0,000

Titration speed

Slower	▲	0
Faster	▼	delay (s)

initial "pH" **1,806**



CurTiPot Distribution Diagrams, Buffer Capacity and Protonation Cur <--- read comment

Plot curves

of the acid/base system

Phosphoric acid

a) as a function of pH and b) overlaid on

Simulated titration curve

Buffer Capacity to be plotted for concentration (mol/L) 1,000000

Acid/base system	
Phosphoric acid	
$pKa_1 = \log K_{pn}$	2,148
$pKa_2 = \log K_{pn-1}$	7,199
$pKa_3 = \log K_{pn-2}$	12,350
$pKa_4 = \log K_{pn-3}$	
$pKa_5 = \log K_{pn-4}$	
$pKa_6 = \log K_{pn-5}$	
Charge of B	-1
pKw	14,000

Overall protonation constants for the pKas	β_p
β_1	2,239E+12
β_2	3,540E+19
β_3	4,977E+21
β_4	
β_5	
β_6	
Protonations	3

Color coding of species in all graphics	
α B	🟥
α HB	⬛
α H_2B	🟩
α H_3B	🟫
α H_4B	🟦
α H_5B	🟪
α H_6B	🟦

Data ID on curves

How to copy/paste a curve

How to change the axis of a curve

Chemistry for Everyone

Analytical Chemistry: A Literary Approach

Charles A. Lucy
Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2, Canada; *charles.lucy@ualberta.ca*

JChemEd.chem.wisc.edu • Vol. 77 No. 4 April 2000 • Journal of Chemical Education **459**

Biblical and Historic Analytical Chemistry

Analytical Chemistry in Classical Mysteries

Modern Analytical Techniques in Best Sellers

Analytical Chemistry in Science Fiction

ac educator

Using Humor To Teach

The right type of humor can help students relate to instructors and material.

Charles A. Lucy
University of Alberta (Canada)

342 A ANALYTICAL CHEMISTRY / JUNE 1, 2002

Does humor enhance learning?
What kinds of humor work?

“Although there is evidence humor works, it is merely a tool…

Making eye contact, calling students by name, moving about the classroom are also effective…

…if humor does not come naturally, it should not be forced.

Teaching Social Responsibility in Analytical Chemistry

M. Valcárcel, G. D. Christian, and R. Lucena, *Anal. Chem.* 2013, **85**, 6152−6161

Concept of Social Responsibility

Corporate Social Responsibilty:

4.- Carroll, A.B. *Business Society*, **1999**, 38, 268-295.

5.-Lindgreen, A.; Swaen, V. Guest Editors of the especial issue on CSR, *J. Management.Rew.*,**2010**, 12, 1-76.

International Standards:

6.- ISO 2600:2010 *Guidance on Social Responsibility*. **2010**, ISO, Genève.

7.- **EFQM framework** on Social Responsibility http://www.efqm.org/en/PdfResources/FrameworkCSR.pdf.

8.- ***Global Reporting Initiative*** (*GRI*) https://www.globalreporting.org/ Pages/ default.aspx.

9.-***SA 8000:2008 standard on Social Accountability***. Social Accountability International, **2008**
http://www.sa-intl.org/.

10.-***United Nations Global Compact*** **2012**, http://www.unglobalcompact.org/.

11.- **OECD guidelines** for multinational enterprises, **2001**
http://www.oecd.org/ investment/guidelinesformultinationalenterprises/1903291.pdf

12.-***Organization Internationale du Travail*** *approach to SR,* **2009**
http://www.ilo.org/empent/Informationresources/WCMS_101253/lang--fr/index.htm.

Definition of SRAC

SRAC can be defined for the chemical information generated as:

- *The awareness of the* ***impact in societal areas*** *(health, agrifood, industry, etc.),*

- *and* ***on the environment****, of the (sustainably) produced chemical knowledge derived from the analysis of natural and artificial objects/samples,*

- *and its* ***correct transmission*** *to circumvent misunderstandings, false expectations and non-justified alarms.*

- *It is related to the* ***ethical principles of the people involved*** *in Analytical Chemistry activities (technicians, analysts/researchers and managers), as well as the recipients of the analytical knowledge.*

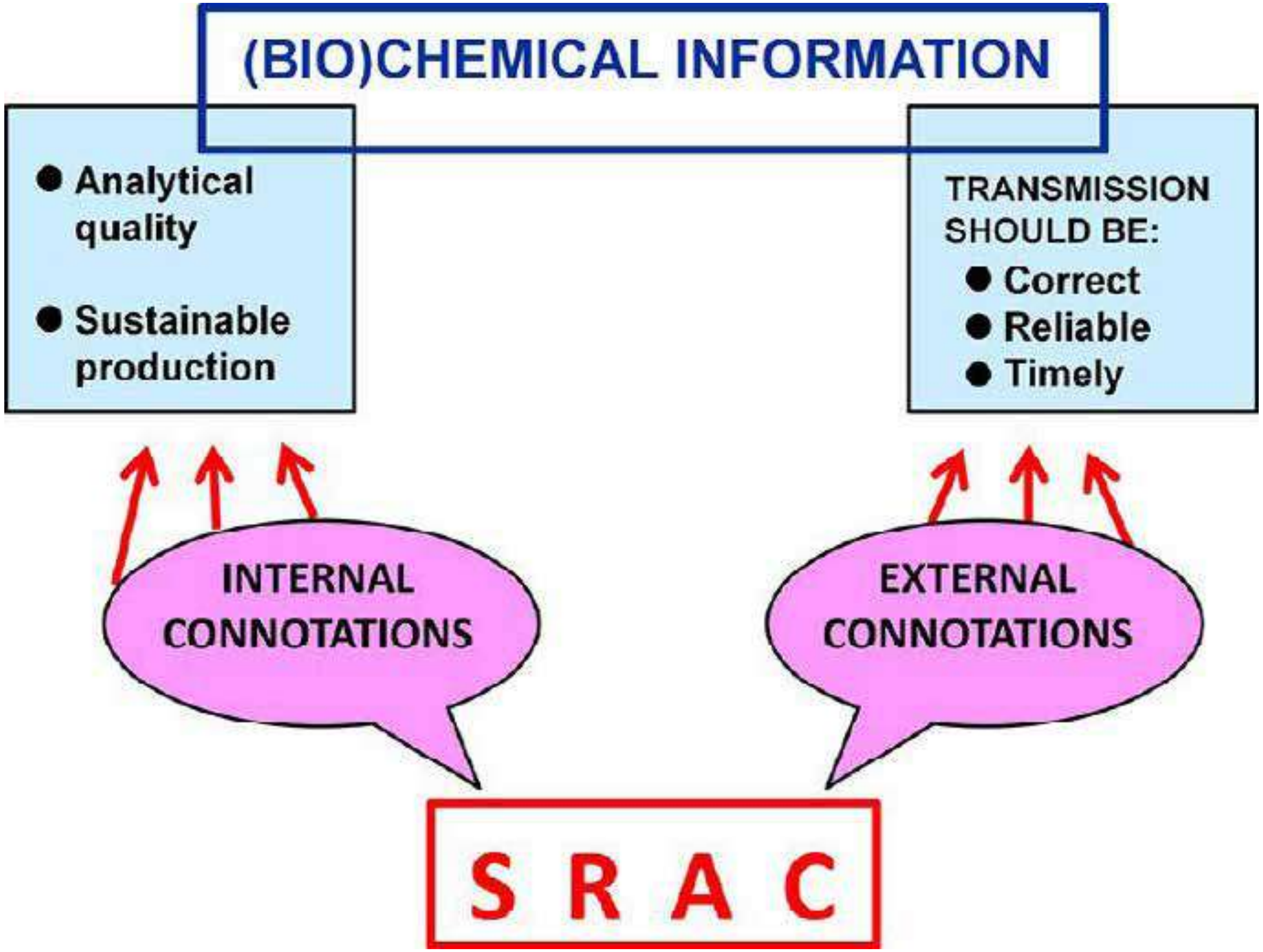


Figure 1. Definition of social responsibility in analytical chemistry (SRAC) based on its internal and external facets.

Internal connotation - **generation of data, to obtain accurate, precise data**

External connotation - **transmission of data:**

- What the results represent (why were they obtained?)
- How well do we know them?
- Important for the end user or for reporting to the public, perhaps by a non-expert.

Internal connotations:

This is really what we teach in the standard analytical chemistry course.
Methods, tools, statistics, etc.

External connotations:

These aspects are less likely to be covered.

Internal connotations:

This is really what we teach in the standard analytical chemistry course.
Methods, tools, statistics, etc.

External connotations:

These aspects are less likely to be covered.

- Analytical courses and texts now may contain a section on
  good laboratory practice
  with emphasis **on validation** of results

- This would be a good place to emphasize the importance of SRAC, highlighting the **importance of accurate analytical information in setting of public policy**.

The analyst must communicate to the requester:

- that careful consideration should be given to **what is requested**
- ask what the **results will be used for**
- and **how well do they need to be known**

The **case study approach** is the most promising way to make the SRAC teaching-learning process more effective.

Recommended:
Students select, present, and discuss examples

Social Responsibility in Publishing

Self-plagiarism
Duplication
Plagiarism
Fabrication
Fraud

Analytical Sciences Digital Library (ASDL)

ASDL Home Portal

Welcome to ASDL

The Analytical Sciences Digital Library

The Analytical Sciences Digital Library, ASDL, collects, catalogs, links and publishes peer reviewed web-based discovery materials pertinent to innovations in curricular development and supporting technical resources in the analytical sciences. The ASDL website (www.asdlib.org) is one of several collections initially funded by NSF's National Science Digital Library (NSDL) program, and is currently supported by the Division of Analytical Chemistry of the American Chemical Society. ASDL grew out of discussions at regional and national meetings on ways to implement recommendations from NSF-sponsored workshops that evaluated teaching practices in the analytical curriculum. These recommendations can be found in the workshop report *Curricular Developments in the Analytical Sciences*, available as a pdf.

Welcome to ASDL!

The ASDL is comprised of four sites: Collection, Community , JASDL, and Active Learning. We hope you will take time to explore each of these sites, and that you find materials or information that are useful in your practice of the analytical sciences. If you find a broken link or other problem, or if you have suggestions to make ASDL better, please contact us. Thanks!

ASDL Associate Editors

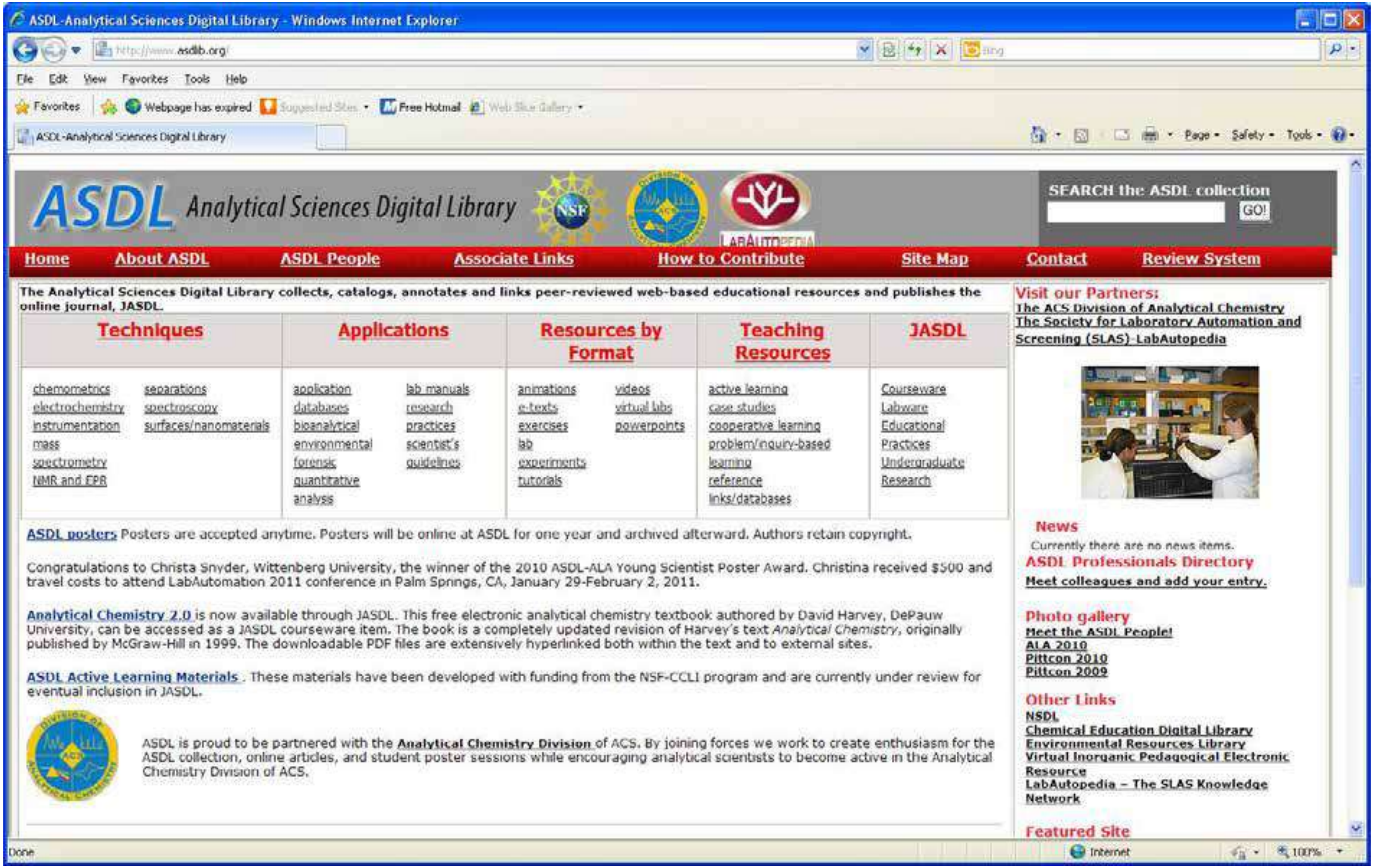
ASDL’s associate editors are the key players in the **peer-review process**.

•Editors take into consideration the reviews that are submitted about each site, then make a determination about accepting the site into the collection.

•At that time the site is annotated and categorized.

Anaytical Sciences Digital Library

www.asdlib.org



The Analytical Sciences Digital Library collects, catalogs, annotates and links peer-reviewed web-based educational resources and publishes the online journal, JASDL.

Techniques	Applications	Resources by Format	Teaching Resources	JASDL
chemometrics electrochemistry instrumentation mass spectrometry NMR and EPR separations spectroscopy surfaces/nanomaterials	application databases bioanalytical environmental forensic quantitative analysis lab manuals research practices scientist's guidelines	animations e-texts exercises lab experiments tutorials videos virtual labs powerpoints	active learning case studies cooperative learning problem/inquiry-based learning reference links/databases	Courseware Labware Educational Practices Undergraduate Research

ASDL posters Posters are accepted anytime. Posters will be online at ASDL for one year and archived afterward. Authors retain copyright.

Congratulations to Christa Snyder, Wittenberg University, the winner of the 2010 ASDL-ALA Young Scientist Poster Award. Christina received $500 and travel costs to attend LabAutomation 2011 conference in Palm Springs, CA, January 29-February 2, 2011.

Analytical Chemistry 2.0 is now available through JASDL. This free electronic analytical chemistry textbook authored by David Harvey, DePauw University, can be accessed as a JASDL courseware item. The book is a completely updated revision of Harvey's text *Analytical Chemistry*, originally published by McGraw-Hill in 1999. The downloadable PDF files are extensively hyperlinked both within the text and to external sites.

ASDL Active Learning Materials . These materials have been developed with funding from the NSF-CCLI program and are currently under review for eventual inclusion in JASDL.

ASDL is proud to be partnered with the **Analytical Chemistry Division** of ACS. By joining forces we work to create enthusiasm for the ASDL collection, online articles, and student poster sessions while encouraging analytical scientists to become active in the Analytical Chemistry Division of ACS.

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LabAutopedia – The SLAS Knowledge Network

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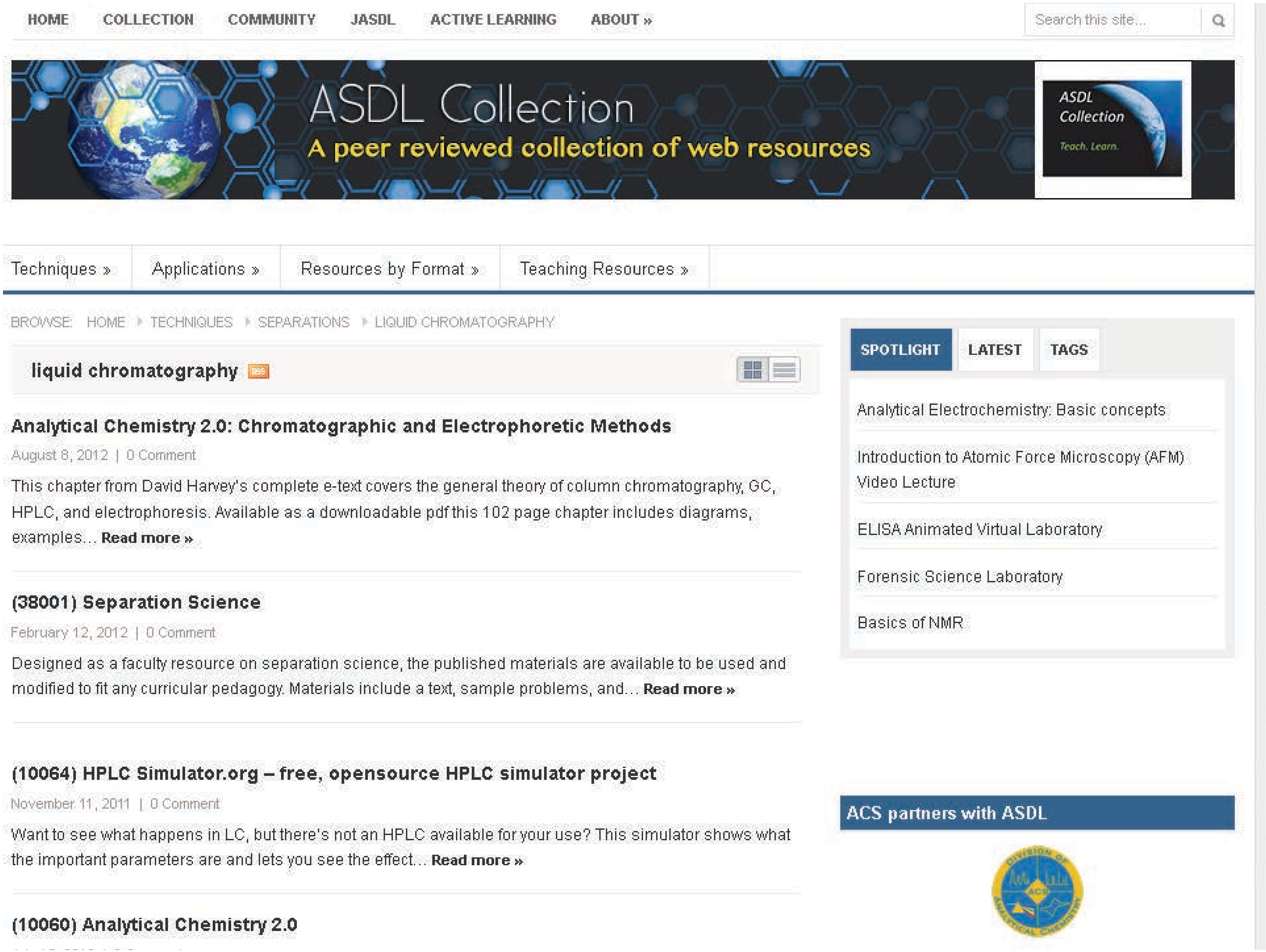

liquid chromatography

Analytical Chemistry 2.0: Chromatographic and Electrophoretic Methods

August 8, 2012 | 0 Comment

This chapter from David Harvey's complete e-text covers the general theory of column chromatography, GC, HPLC, and electrophoresis. Available as a downloadable pdf this 102 page chapter includes diagrams, examples… **Read more »**

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Designed as a faculty resource on separation science, the published materials are available to be used and modified to fit any curricular pedagogy. Materials include a text, sample problems, and… **Read more »**

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November 11, 2011 | 0 Comment

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(10060) Analytical Chemistry 2.0

Analytical Electrochemistry: Basic concepts

Introduction to Atomic Force Microscopy (AFM) Video Lecture

ELISA Animated Virtual Laboratory

Forensic Science Laboratory

Basics of NMR

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HPLC Simulator.org – free, opensource HPLC simulator project

Want to see what happens in LC, but there's not an HPLC available for your use? This simulator shows what the important parameters are and lets you see the effect of changing those parameters on realistic separations.

The website is available here .

Leave a Reply

SPOTLIGHT LATEST TAGS

Analytical Electrochemistry: Basic concepts

Introduction to Atomic Force Microscopy (AFM) Video Lecture

ELISA Animated Virtual Laboratory

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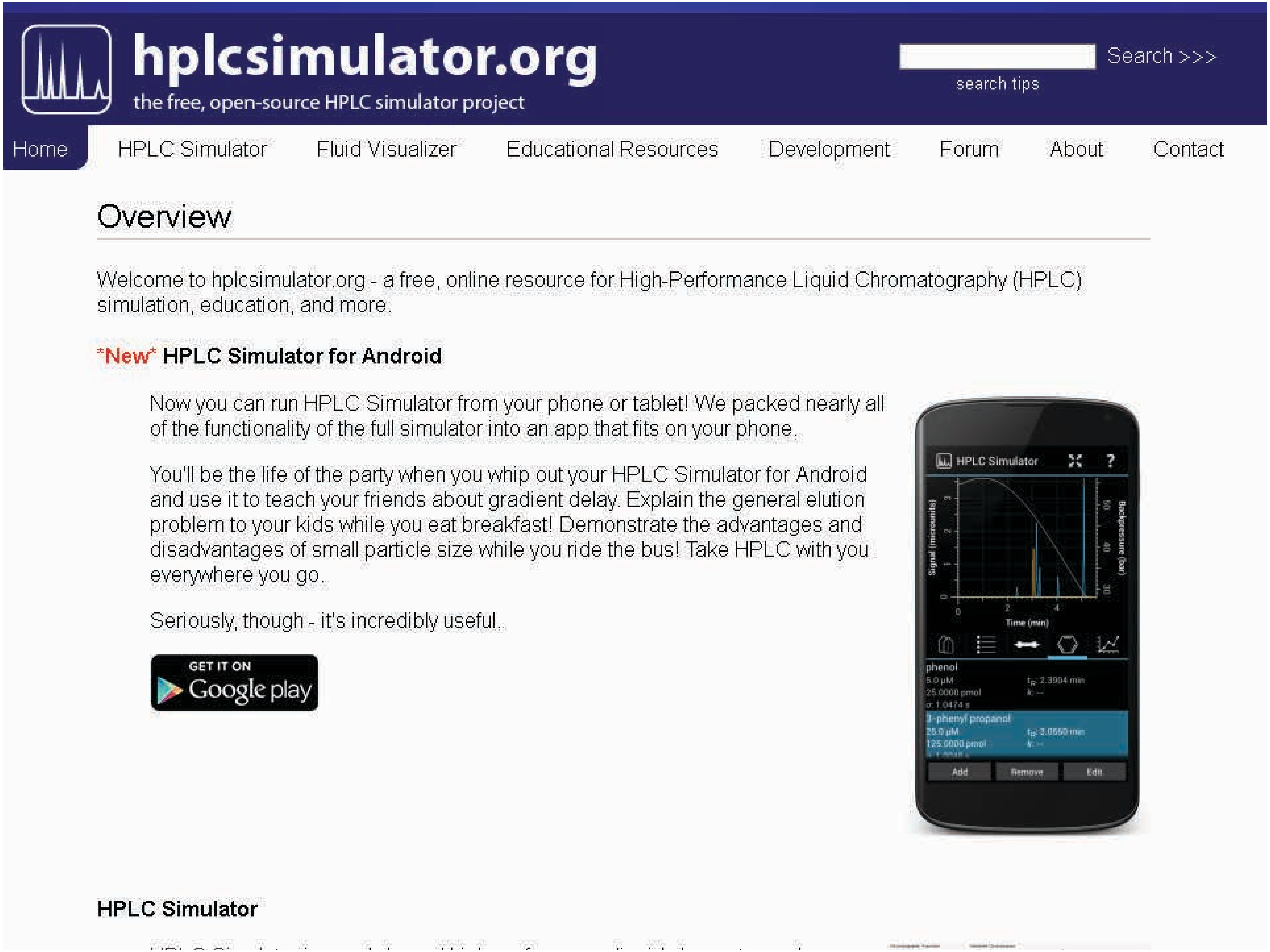


Overview

Welcome to hplcsimulator.org - a free, online resource for High-Performance Liquid Chromatography (HPLC) simulation, education, and more.

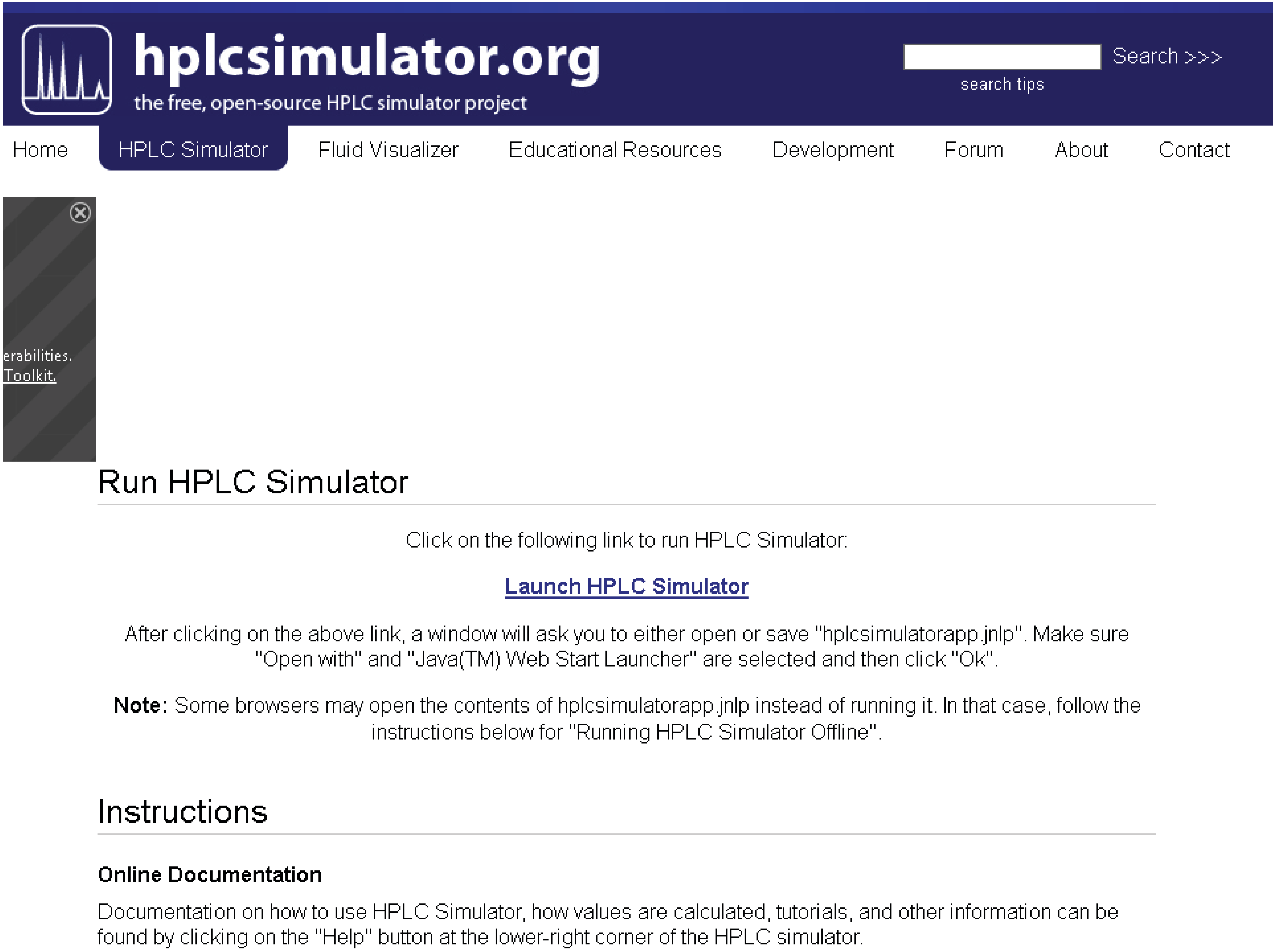
New HPLC Simulator for Android

Now you can run HPLC Simulator from your phone or tablet! We packed nearly all of the functionality of the full simulator into an app that fits on your phone.

You'll be the life of the party when you whip out your HPLC Simulator for Android and use it to teach your friends about gradient delay. Explain the general elution problem to your kids while you eat breakfast! Demonstrate the advantages and disadvantages of small particle size while you ride the bus! Take HPLC with you everywhere you go.

Seriously, though - it's incredibly useful.

HPLC Simulator



Run HPLC Simulator

Click on the following link to run HPLC Simulator:

Launch HPLC Simulator

After clicking on the above link, a window will ask you to either open or save "hplcsimulatorapp.jnlp". Make sure "Open with" and "Java(TM) Web Start Launcher" are selected and then click "Ok".

Note: Some browsers may open the contents of hplcsimulatorapp.jnlp instead of running it. In that case, follow the instructions below for "Running HPLC Simulator Offline".

Instructions

Online Documentation

Documentation on how to use HPLC Simulator, how values are calculated, tutorials, and other information can be found by clicking on the "Help" button at the lower-right corner of the HPLC simulator.

Some conclusions:

- Teach students the relevance of AC in society
- Teach some history
- Teach the importance of what is reported
- Teach what questions to ask in requests for analyses
- Teach how to get a representative & meaningful sample
- Revaluate what is taught
    - What is actually used?
    - Bring in industrial partners
- But don't ignore classical topics
    - Mastering equilibria is important in many disciplines
    - Laboratory experiments should teach careful techniques
- Accommodate different student learning skills
- Utilize new technologies
- Teach communication skills!
    - written
    - oral

Lord Kelvin

(William Thompson, 1824-1907)

“Unless our knowledge is measured in numbers, it does not amount to much”

Thank you – And happy teaching!