Electronic Distribution of Science Publications

A Learn in 30

OPCUG & PATACS

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Outline

- How scientists communicate
- Science journals
- Example journal article
- Printing and electronic delivery
- The publishing process
- Creation of paper and electronic journals
- Challenges to electronic publishing
- Cooperative experiments
- Success!

How Do Scientists Communicate?

- Personal contact and human networking
- Conferences and formal meetings
- Abstracting/Indexing services
  - ✓ STN International (~150 databases) and SciFinder
  - ✓ ISI (International Scientific Indexing)
  - ✓ MEDLINE (NLM/NIH)
- Patents (worldwide)
- **Science Journals** (worldwide)

What Is a Journal?

- The dominant means of communicating science—**the historical record**
- Articles written by active scientists (not journalists)
- Articles highly structured, technical and detailed
- Articles screened by a journal editor (scientist)
- Submitted manuscripts are peer reviewed
- In STM—English dominate language

Of ~~the~~ A Way of killing Ratle-Snakes.

There being not long ſince occaſion given at a meeting of the *Royal Society* to diſcourſe of *Ratle-Snakes*, that worthy and inquiſitive Gentleman, Captain *Silas Taylor*, related the manner, how they were killed in *Virginia*, which he afterwards was pleaſed to give in writing, atteſted by two credible perſons in whoſe preſence it was don; which is, as follows.

The Wild *Penny-royal* or *Ditany* of *Virginia*, groweth ſtreight up about one foot high, with the leaves like *Penny royal*, with little blue tufts at the joyning of the branches to the Plant, the colour of the Leaves being a reddiſh green, but the Water diſtilled, of the colour of Brandy, of a fair Yellow: the Leaves of it bruiſed are very hot and biting upon the Tongue: and of theſe, ſo bruiſed, they took ſome, and having tyed them in the cleft of a long ſtick, they held them to the Noſe of the *Ratle-Snake*, who by turning and wriggling laboured as much as ſhe could to avoid it: but ſhe was killed with it, in leſs than half an hour's time, and, as was ſuppoſed, by the ſcent thereof; which was done *Anno* 1657. in the Month of *July*, at which ſeaſon, they repute thoſe creatures to be in the greateſt vigour for their poiſon.

From the *Philosophical Transactions of the Royal Society,* vol 1, March 1665
[First science journal: Journal des sçavans (January 1665)]

Chemistry Journals

- ~ 1,500 journals of interest to chemists
- ~ 95% published by commercial publishers
- ~ 5% published by not-for-profit organizations
  - ✓ European Chemical Society (50 member societies*)
  - ✓ The Royal Society of Chemistry—44 journals
  - ✓ Gesellschaft Deutscher Chemiker—10 journals
  - ✓ American Chemical Society—75 journals

* American Chemical Society (ACS) is an affiliate member

ACS Journals: 36 of 75

ACS Journals: another 36 of 75

Journal Title →

VOLUME 37 NUMBER 3

ACCOUNTS of CHEMICAL RESEARCH®

MARCH 2004

Title →

Communicating Original Research in Chemistry and Related Sciences

Author →

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Received August 1, 2003

Abstract →

ABSTRACT
The availability of scientific information in electronic form is the convergence of traditional journal publishing, electronic communications, and the widespread availability of computer technology. This revolution in scientific communication has its roots in developments that started in the mid-19th century and culminated with the extraordinary progress in telecommunications and computer technology in the latter years of the 20th century. Eighty-three percent of scientific journals are now available online. The benefits of electronic journals include rapid publication, instantaneous linking to external information sources, and the capability to deliver new types of information. To date neither electronic-only nor preprint servers have been well received by the chemical sciences community. Continued advances in telecommunications, computer technology, and acquisition of scientific data in structured formats hold promise for even greater advances in communication of scientific information.

munication channels—printed scientific journals and electronic communications—plus widespread availability of inexpensive computer technology. The first two printed scientific journals were published in 1665, the French journal *Journal des Scavans* and the British publication *Philosophical Transactions*. Electronic communications and the development of computers have an earlier history than is often appreciated.

- 1843—patent for FAX was awarded to Alexander Bain.
- 1844—Samuel Morse installed a telegraph line between Baltimore, Maryland, and Washington, DC.
- 1876—Alexander Graham Bell patented the telephone.
- 1890—Herman Hollerith was awarded a contract for processing the 1890 U.S. census using punched cards.
- 1924—Hollerith's Tabulating Machine Company becomes IBM.
- 1941—Konrad Zuse developed the first programmable calculator using binary numbers and Boolean logic.
- 1964—IBM released the IBM model 360 mainframe computer.
- 1965—Digital Equipment Corporation (DEC) introduced

Discussion

In 1980, the American Chemical Society, in cooperation with Chemical Abstracts Service and BRS, made available a databas[...] *dicinal Chemistr*[...]ch was arguably [...]ailable online. In [...] made available [...]he ACS journals were made available through STN International, as were selected journals from Elsevier, John Wiley & Sons, the Royal Society of Chemistry (RSC) and others. These implementations suffered serious defects that limited their adoption and use. Only ASCII characters were permitted; thus, for example, the α character was represented by the string ".alpha.". Tabular material was unavailable as were graphic data, thus excluding line art, half-tones, and color. Even if graphics had been available, the slow speed of dial-up telecommunications at the time would have made downloading impractical. Despite the lack of success with these endeavors, experience gained in creating these systems was very valuable in traveling the road to the World Wide Web.

During 1989–1995, the ACS Publications Division, Bellcore, Chemical Abstracts Service, Cornell University, and Online Computer Library Center (OCLC) collaborated in what became known as the CORE project.[4,5] This was an effort to create a prototype digital library at Cornell University using the ACS journals as the data source and software from OCLC as the user interface and back-end system. In 1992–1997, the ACS participated with approximately 20 other publishers in the Red Sage Project to create a prototype electronic library at the University of California at San Francisco.[6,7] In the Red Sage Project, RightPages software from Bell Laboratories was used for the user interface and underpinning data structures. Both

1433. In a recent survey of 275 journal publishers, Cox and Cox[9] have reported that of the scientific, technical, and medical (STM) titles, 83% are available online.

Notable Players in Electronic Publishing

Unquestionably, the age of electronic dissemination of scientific information has arrived and is an integral part of STM publishing. Most STM publishers now deliver both print and Web products and provide Web-based manuscript submission systems for their authors.

Elsevier is the largest commercial publisher in science and offers an increasingly integrated line of products. Elsevier's journals are available through a variety of purchase plans through Science Direct. Science Direct is linked to Elsevier's Scirus, a free "Google-like" search engine for the sciences. Elsevier's ChemWeb is a portal for chemistry and is tightly coupled with Elsevier's preprint server. Elsevier's MDL, a software company that largely focuses on the drug discovery market, is also associated with CrossFire Beilstein.

At the other end of the business model spectrum lies the Public Library of Science (PLoS). This is a venture in which it is proposed authors, rather than journal purchasers, would financially support the publishing enterprise by paying a $1500 per manuscript fee. The production cost per manuscript for ACS journals in 2002 was $1544 exclusive of paper, printing, and distribution,[10] which is remarkably close to PLoS's $1500 fee. PLoS was established in October 2000 as a nonprofit organization and has its roots in a protest movement originating at Stanford University in which scientists were asked to boycott those publishers that would not allow unrestricted free access to their journal articles six months after publication.

Graphics (B&W)

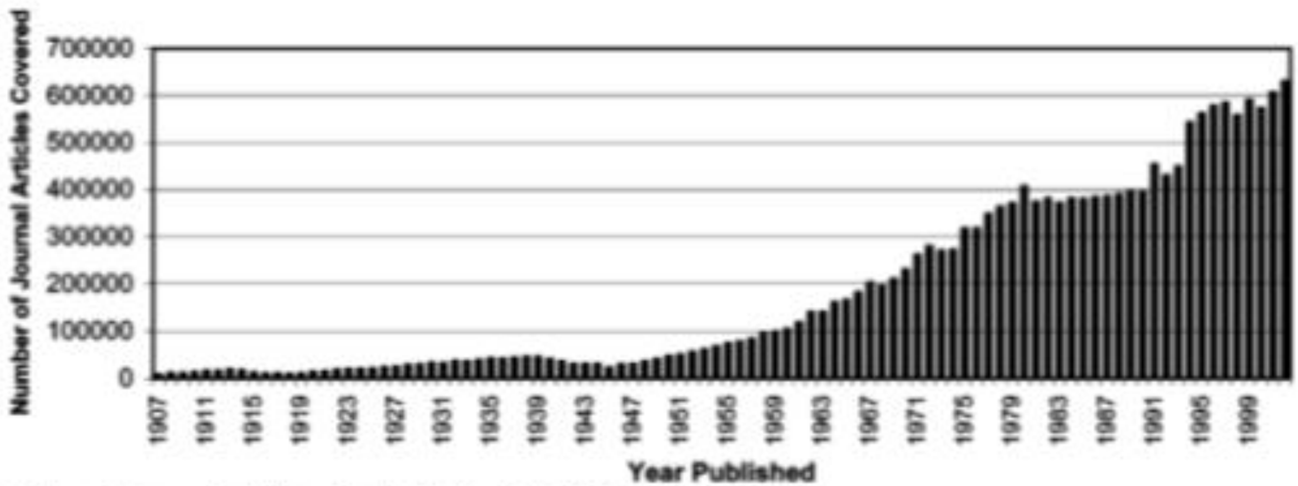

FIGURE 3. Journal Articles Covered in *Chemical Abstracts*, 1907–2002.

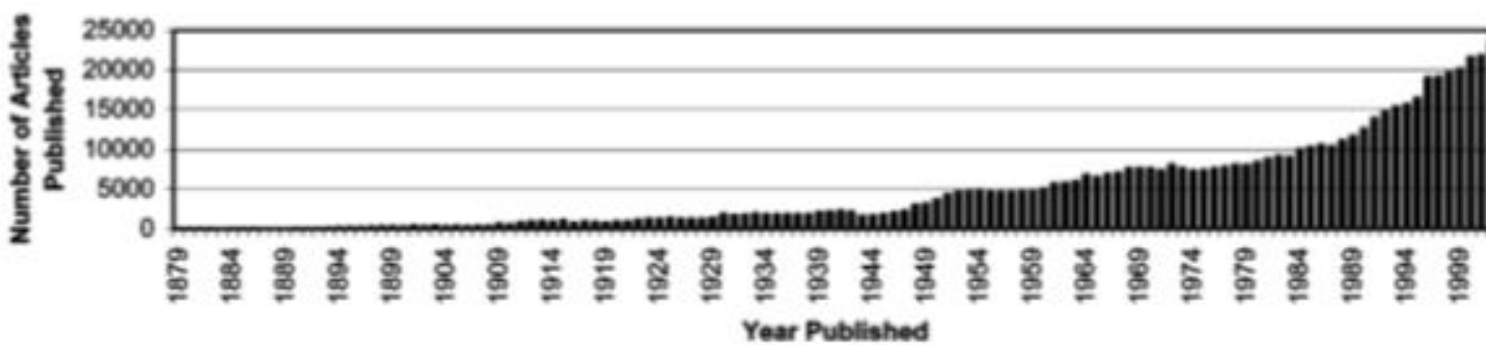

FIGURE 4. Journal Articles Published by the ACS, 1879–2002.

thermodynamic[...]
of the journal
scientific data in
prepares a man[...]

References

significantly enrich the value of such papers and make the creation of secondary databases more efficient and complete. Some progress has been made to encode chemical information in extensible markup language (XML) as CML (chemical markup language) by Murray-Rust and Rzepa.[63−68] However, there is much more work to be done, and authoring software tools are yet to be developed.

Efforts are also being made to develop data format standards in XML for analytical instruments. The standards group ASTM E13.15 is attempting to develop a specification for a common core of elements in XML format that would address data interchange and archiving issues that could be used across all analytical techniques (MS, NMR, IR, gas chromatography, etc.). This core specification is known as AnIML (analytical information markup language). Subsequently instrument-specific specifications will be developed. In time, these XML specifications are likely to replace the current Joint Committee on Atomic and Molecular Physical Data (JCAMP) standards.[69]

The Future

Considering that electronic journal publishing is less than 10 years old and the remarkable progress that has been made in this short time, we can expect many exciting advances to come in the years ahead. The costs for publishing large data sets and extensive experimental details by traditional means are mostly reduced by

References

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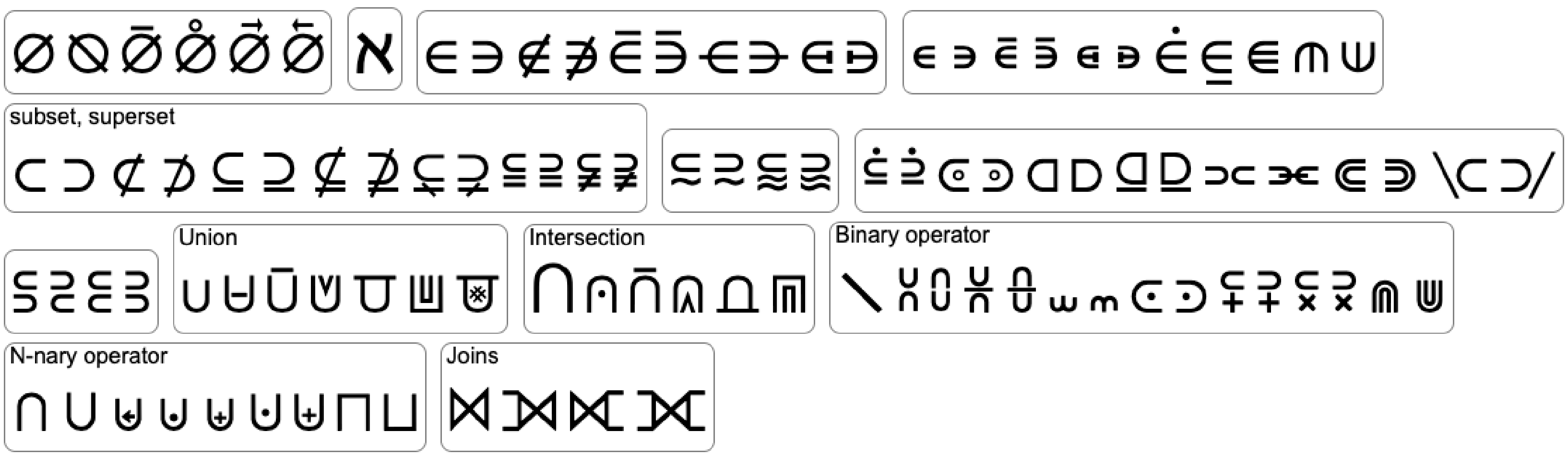
Articles Often Also Contain…

Special Characters

Greek Alphabet

ΑΒΓΔΕΖΗΘΙΚΛΜΝΞΟΠΡΣΤΥΦΧΨΩ
αβγδεζηθικλμνξοπρστυφχψω



Special Characters (cont.)

Precede / succeed

≺ ≻ ≼ ≽ ≾ ≿ ⊀ ⊁ ⋞ ⋟ ⋠ ⋡ ⋨ ⋩ ⪯ ⪰ ⪱ ⪲ ⪳ ⪴ ⪵ ⪶ ⪷ ⪸ ⪹ ⪺ ⪻ ⪼ ⊰ ⊱

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+approx

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+equivalence

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+similarity

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Identity

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Equivalence

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asymptotic

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Misc relations

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Normal subgroups

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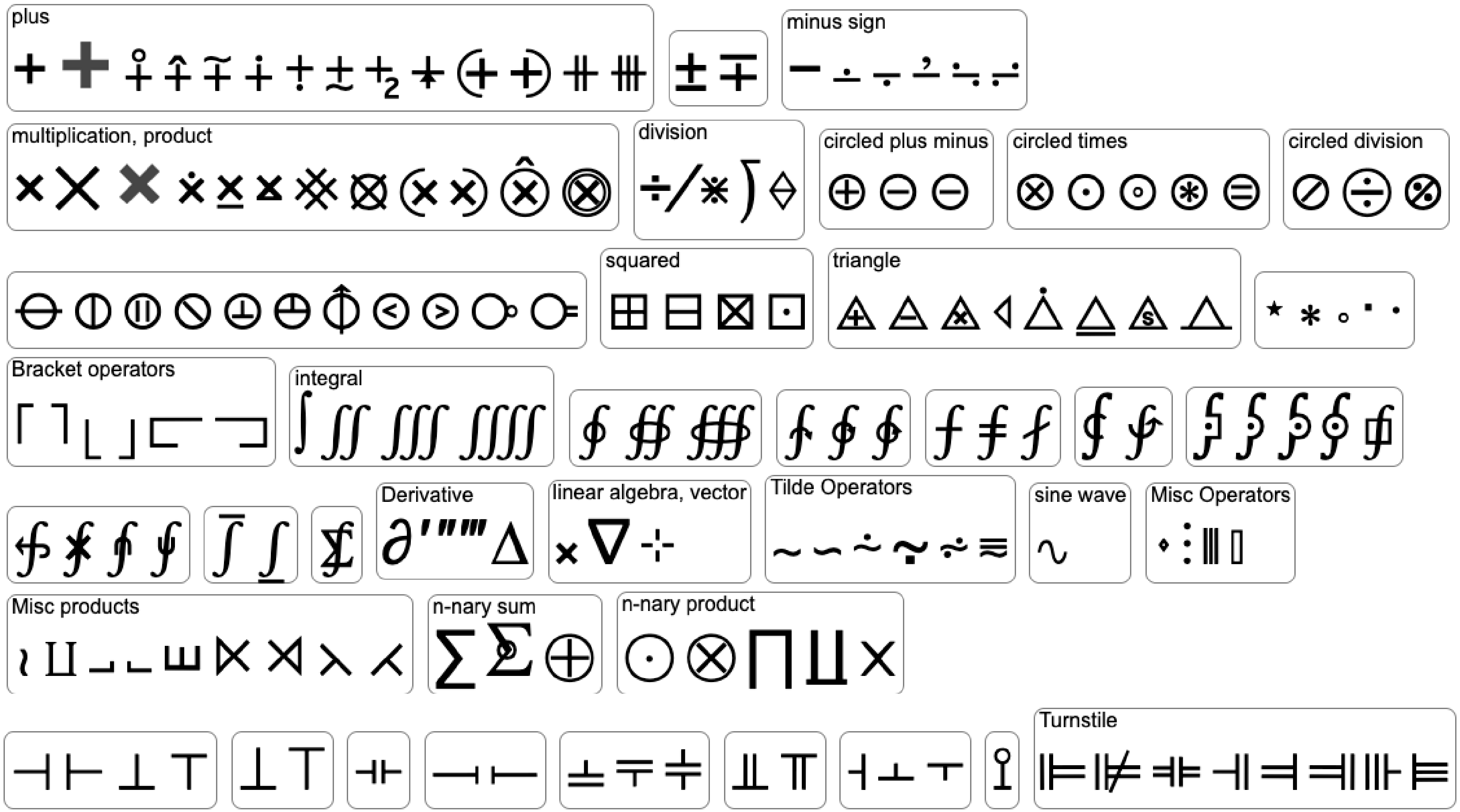
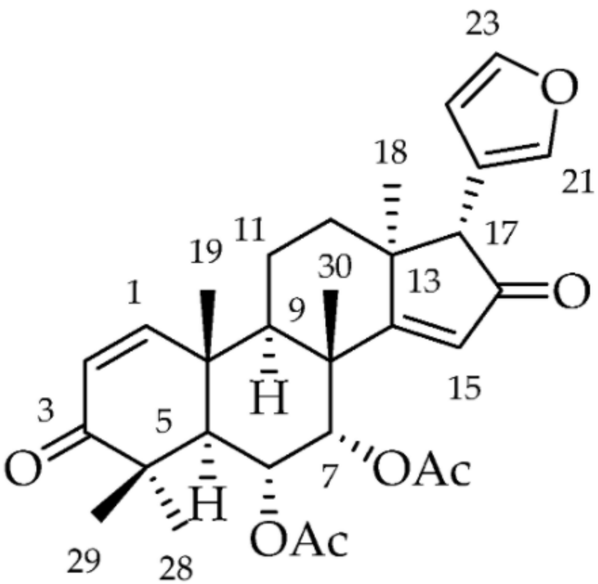
Special Characters (cont.)

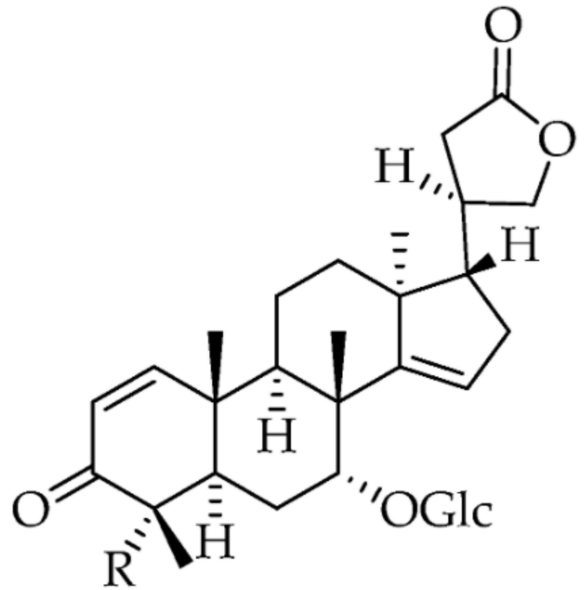


And many more…

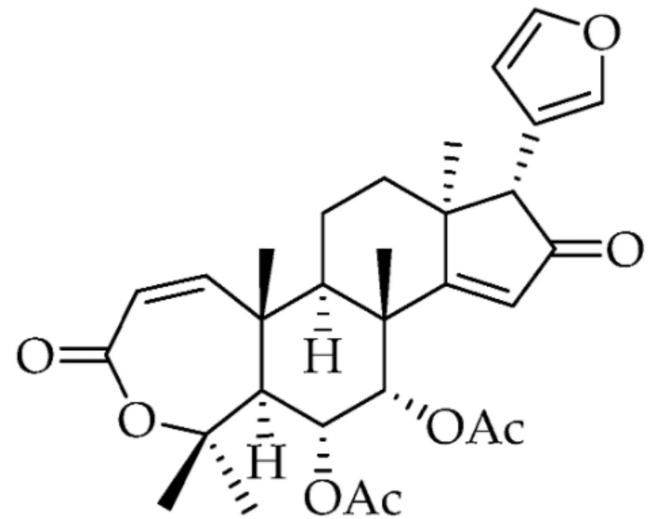
Chemical Structures



1 mahonin



2 swieteliacate A R=H
3 swieteliacate B R=OH

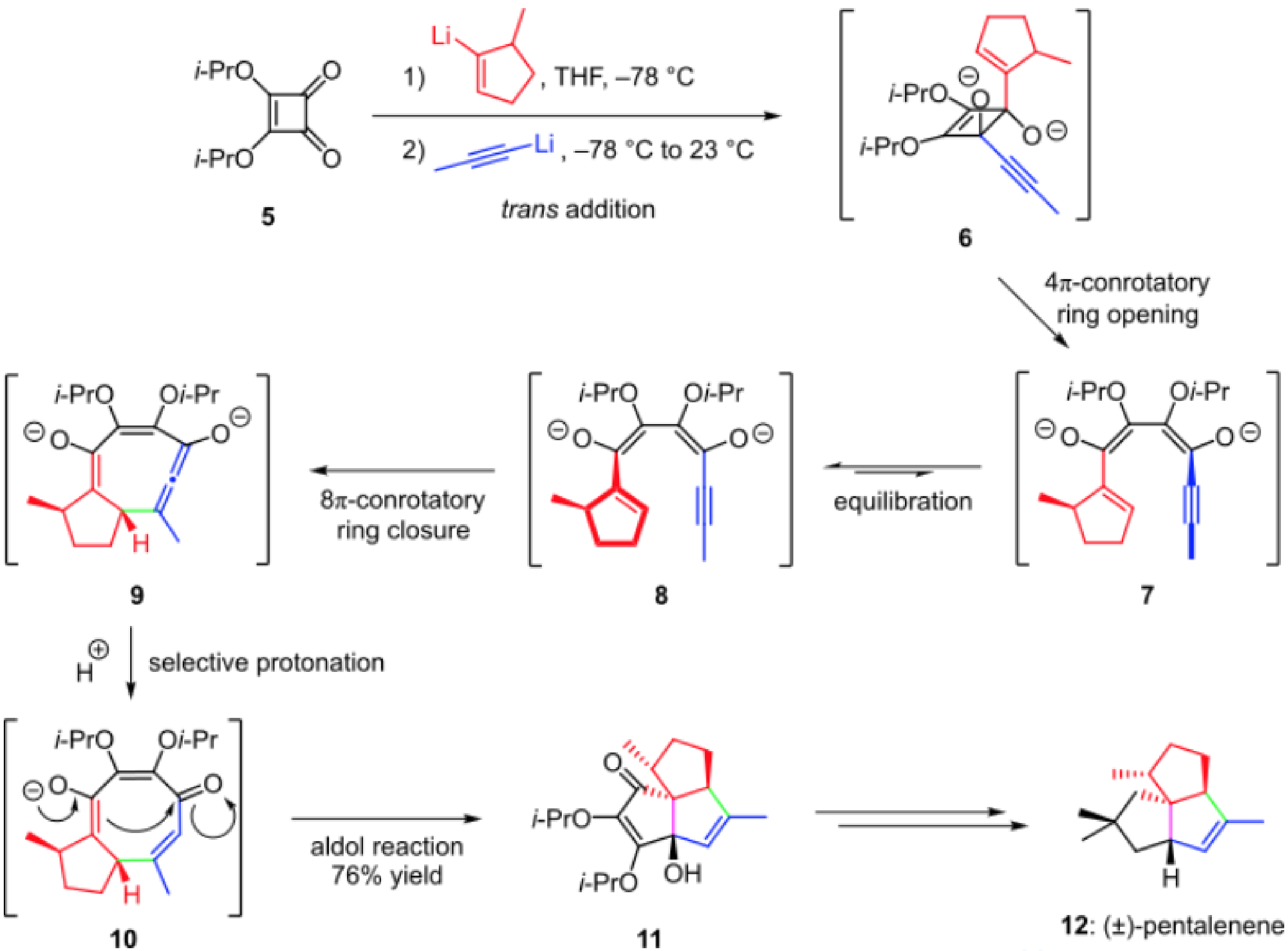


4 swimacronoid A

Historically drawn by hand
Keyboarded by highly skilled staff
Created using software

Information retrievable by structure and sub-structure searching (181+ million substances)

Chemical Reaction Sequences



Scheme 2. Cascade reaction in the total synthesis of (±)-pentalenene[4]

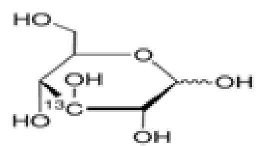
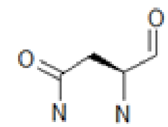
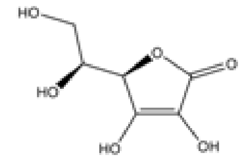
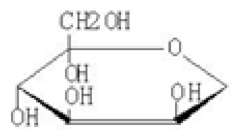
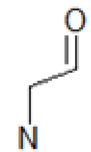
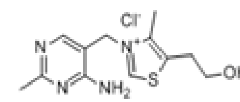
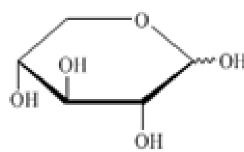
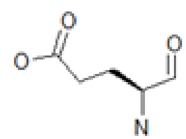
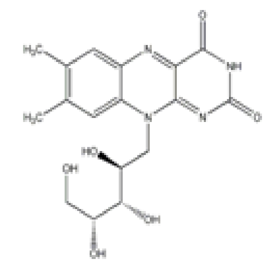
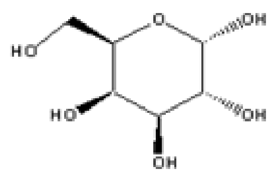
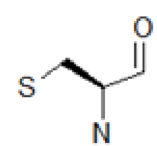
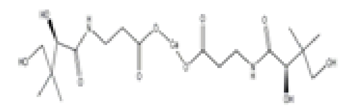
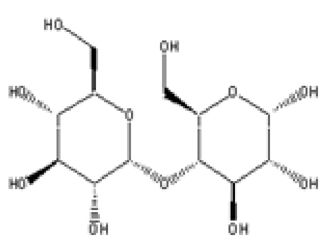
Tables

Compound	Kp (equation 1)							Mean
	1	2	3	4	5	6	7	
Epigallocatechin gallate	$1.42\cdot10^{-6}$	$7.84\cdot10^{-6}$	$4.76\cdot10^{-7}$	$2.53\cdot10^{-6}$	$5.02\cdot10^{-7}$	$4.66\cdot10^{-6}$	$3.43\cdot10^{-6}$	$2.98\cdot10^{-6}$
Epicatechin gallate	$4.38\cdot10^{-6}$	$1.98\cdot10^{-5}$	$1.46\cdot10^{-6}$	$5.15\cdot10^{-6}$	$2.56\cdot10^{-6}$	$1.43\cdot10^{-5}$	$5.84\cdot10^{-6}$	$7.65\cdot10^{-6}$
Epigallocatechin	$1.42\cdot10^{-5}$	$5.19\cdot10^{-5}$	$4.05\cdot10^{-6}$	$6.95\cdot10^{-6}$	$1.54\cdot10^{-6}$	$3.08\cdot10^{-5}$	$1.45\cdot10^{-5}$	$1.77\cdot10^{-5}$
Gallocatechin	$1.42\cdot10^{-5}$	$5.19\cdot10^{-5}$	$4.05\cdot10^{-6}$	$6.95\cdot10^{-6}$	$1.54\cdot10^{-6}$	$3.08\cdot10^{-5}$	$1.45\cdot10^{-5}$	$1.77\cdot10^{-5}$
Catechin	$4.38\cdot10^{-5}$	$1.31\cdot10^{-4}$	$1.25\cdot10^{-5}$	$1.85\cdot10^{-5}$	$7.68\cdot10^{-6}$	$9.32\cdot10^{-5}$	$2.47\cdot10^{-5}$	$4.74\cdot10^{-5}$
Gallocatechin gallate	$1.42\cdot10^{-6}$	$7.84\cdot10^{-6}$	$4.76\cdot10^{-7}$	$2.53\cdot10^{-6}$	$5.02\cdot10^{-7}$	$4.66\cdot10^{-6}$	$3.43\cdot10^{-6}$	$2.98\cdot10^{-6}$
Theaflavine	$3.63\cdot10^{-9}$	$2.15\cdot10^{-8}$	$3.63\cdot10^{-9}$	$5.67\cdot10^{-8}$	$1.03\cdot10^{-8}$	$2.47\cdot10^{-7}$	$2.22\cdot10^{-7}$	$8.07\cdot10^{-8}$
Theaflavine 3-gallate	$3.63\cdot10^{-10}$	$3.25\cdot10^{-9}$	$4.26\cdot10^{-10}$	$8.41\cdot10^{-9}$	$3.43\cdot10^{-9}$	$3.80\cdot10^{-8}$	$5.25\cdot10^{-8}$	$1.52\cdot10^{-8}$
Theaflavine 3'-gallate	$3.63\cdot10^{-10}$	$3.25\cdot10^{-9}$	$4.26\cdot10^{-10}$	$8.41\cdot10^{-9}$	$3.43\cdot10^{-9}$	$3.80\cdot10^{-8}$	$5.25\cdot10^{-8}$	$1.52\cdot10^{-8}$
Theaflavine 3.3'-digallate	$1.12\cdot10^{-10}$	$1.24\cdot10^{-9}$	$1.54\cdot10^{-10}$	$1.28\cdot10^{-9}$	$1.05\cdot10^{-9}$	$1.77\cdot10^{-8}$	$5.40\cdot10^{-9}$	$3.84\cdot10^{-9}$
Kempferol	$1.25\cdot10^{-5}$	$2.25\cdot10^{-5}$	$7.64\cdot10^{-5}$	$1.18\cdot10^{-4}$	$1.43\cdot10^{-4}$	$2.29\cdot10^{-4}$	$1.11\cdot10^{-4}$	$1.02\cdot10^{-4}$
Quercetin	$4.05\cdot10^{-6}$	$8.76\cdot10^{-6}$	$2.48\cdot10^{-5}$	$5.57\cdot10^{-5}$	$3.19\cdot10^{-5}$	$7.56\cdot10^{-5}$	$3.08\cdot10^{-5}$	$3.31\cdot10^{-5}$
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 3. The values of log Kp for selected theafl avonoids calculated according equation (1).

Tables

Journal of Food and Nutrition Research. **2014**, 2(7), 344-348 doi:10.12691/jfnr-2-7-3

Type	Chemical structure formula	Type	Chemical structure formula	Type	Chemical structure formula
L-glucose (GLU)		L-asparagine (Asn)		L-ascorbic acid (VC)	
fructose (Fru)		L-glycine (Gly)		thiamin (VB_1)	
D-xylose (Xyl)		L-glutamic acid (Glu)		riboflavin (VB_2)	
galactose (Gal)		L-cysteine (Cys)		calcium pantothenate (VB_5)	
Maltose (Mal)					

Complex Mathematics

$$\dot{p} = \sqrt{\frac{p}{\mu}} \frac{2p}{w} \frac{T}{m} \alpha_t$$

$$\dot{f} = \sqrt{\frac{p}{\mu}} \left[\sin L \frac{T}{m} \alpha_r + \frac{(1+w)\cos L + f}{w} \frac{T}{m} \alpha_t - \frac{(h \sin L - k \cos L) g}{w} \frac{T}{m} \alpha_n \right]$$

$$\dot{g} = \sqrt{\frac{p}{\mu}} \left[-\cos L \frac{T}{m} \alpha_r + \frac{(1+w)\sin L + g}{w} \frac{T}{m} \alpha_t + \frac{(h \sin L - k \cos L) f}{w} \frac{T}{m} \alpha_n \right]$$

$$\dot{h} = \sqrt{\frac{p}{\mu}} \frac{s^2 \cos L}{2w} \frac{T}{m} \alpha_n$$

$$\dot{k} = \sqrt{\frac{p}{\mu}} \frac{s^2 \sin L}{2w} \frac{T}{m} \alpha_n$$

$$\dot{L} = \sqrt{\mu p} \left(\frac{w}{p} \right)^2 + \sqrt{\frac{p}{\mu}} \frac{h \sin L - k \cos L}{w} \frac{T}{m} \alpha_n$$

Photographs (B&W)

Figure 1

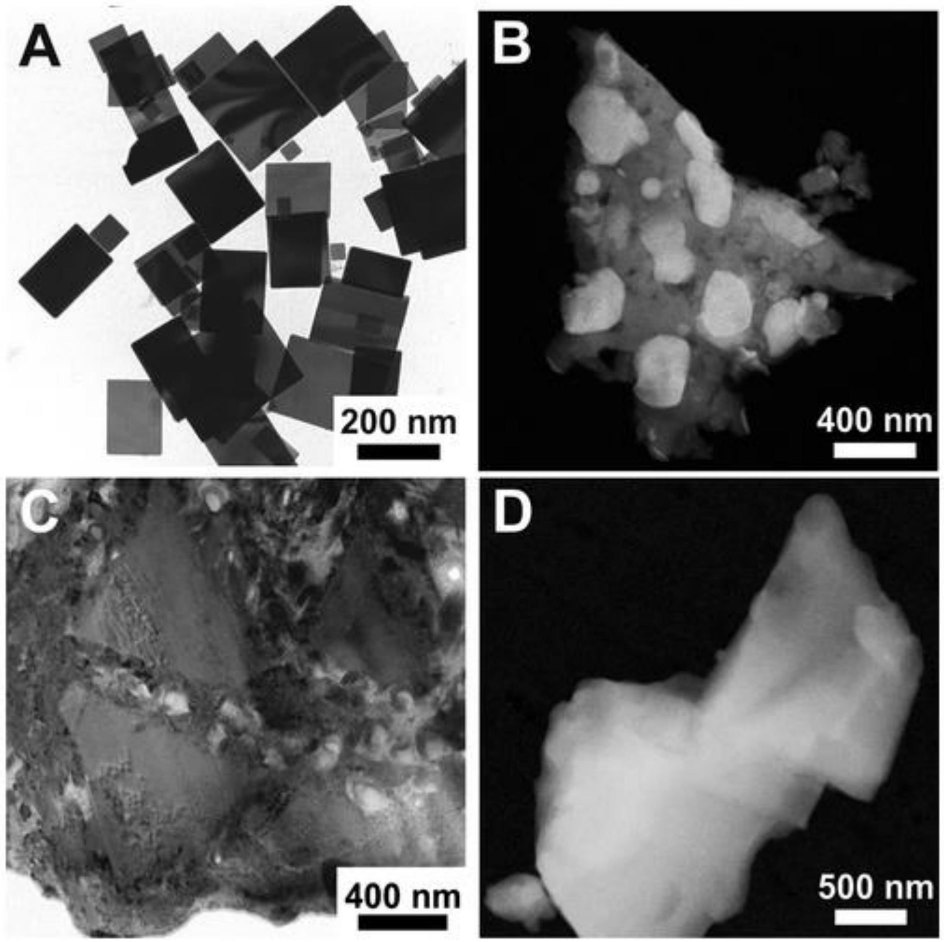
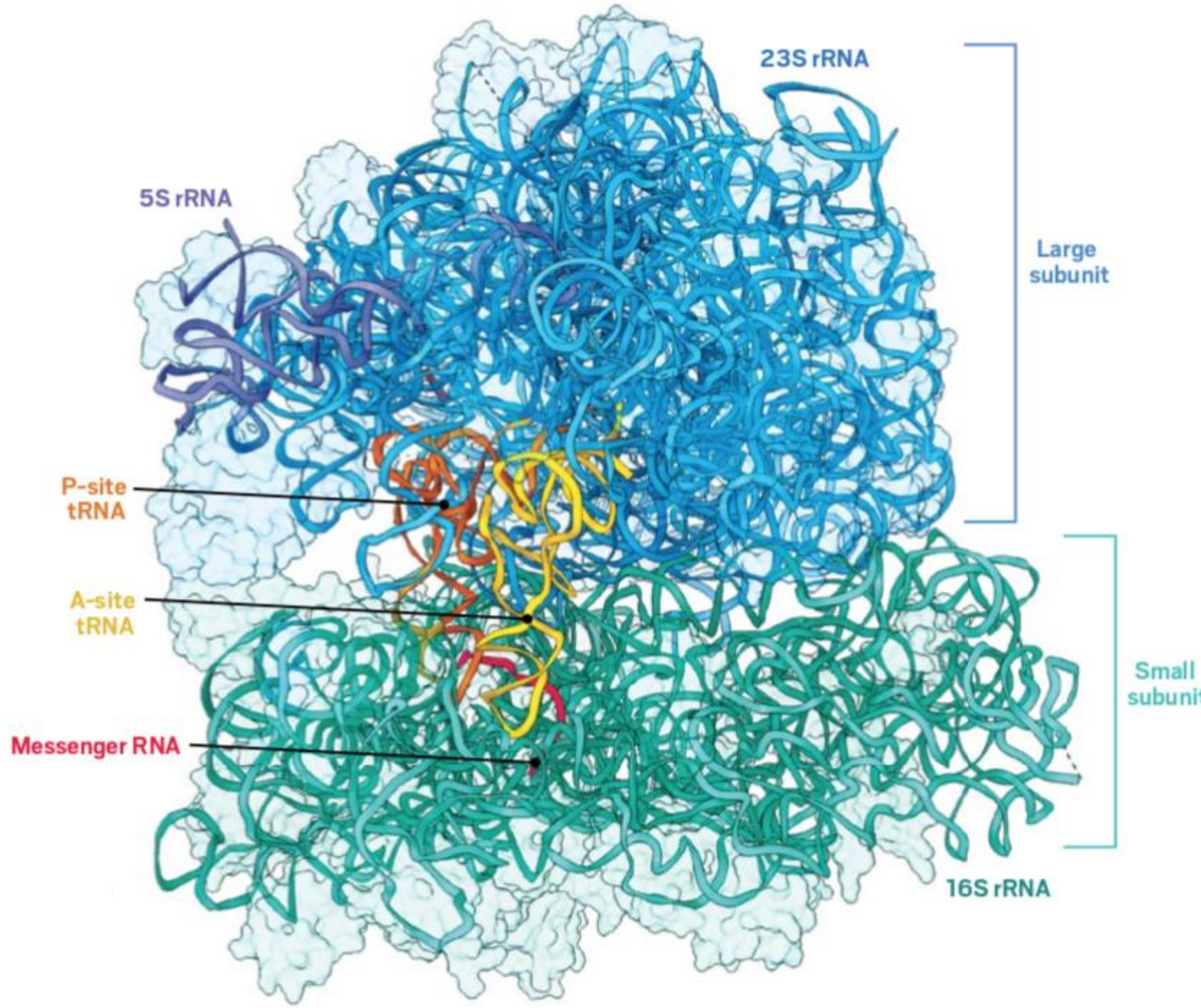


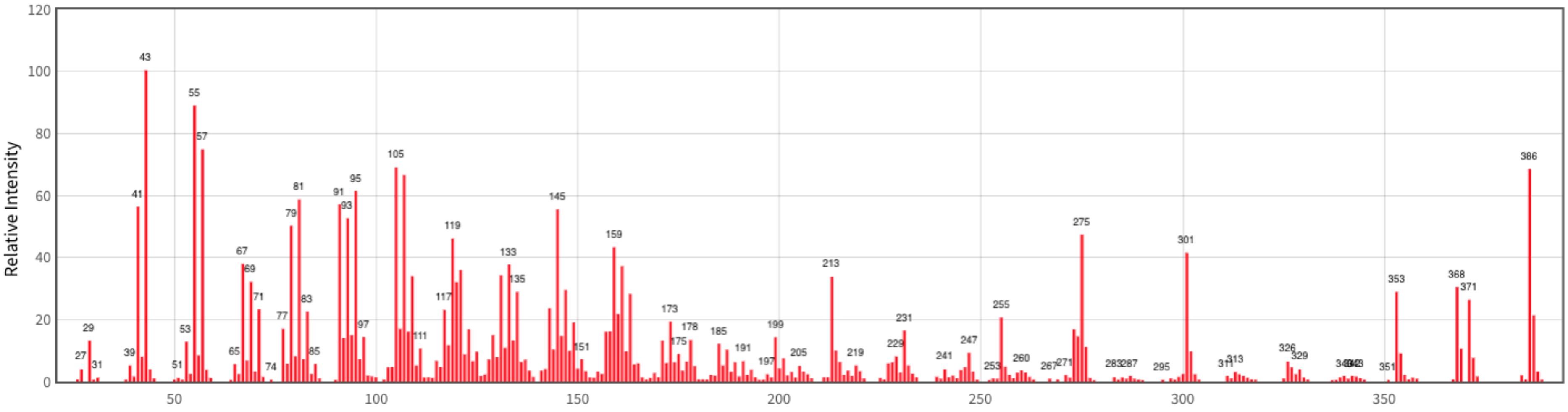
Figure 1. Examples of crystals suitable for 3D ED data collection. (A) $Cu_{2-x}Te$ nanoplatelets, with lateral size of 100–200 nm and thickness of few tens of nanometers. (B) Submicrometric $Eu_2Si_2O_7$ grains embedded in a ground mass of nanocrystalline quartz. (C) Submicrometric cronstedtite pyramidal crystals in a focused ion beam (FIB) lamella, sampled from the carbonaceous meteorite Paris. (D) Micrometric pharmaceutical crystal.

Complex Molecules and Color

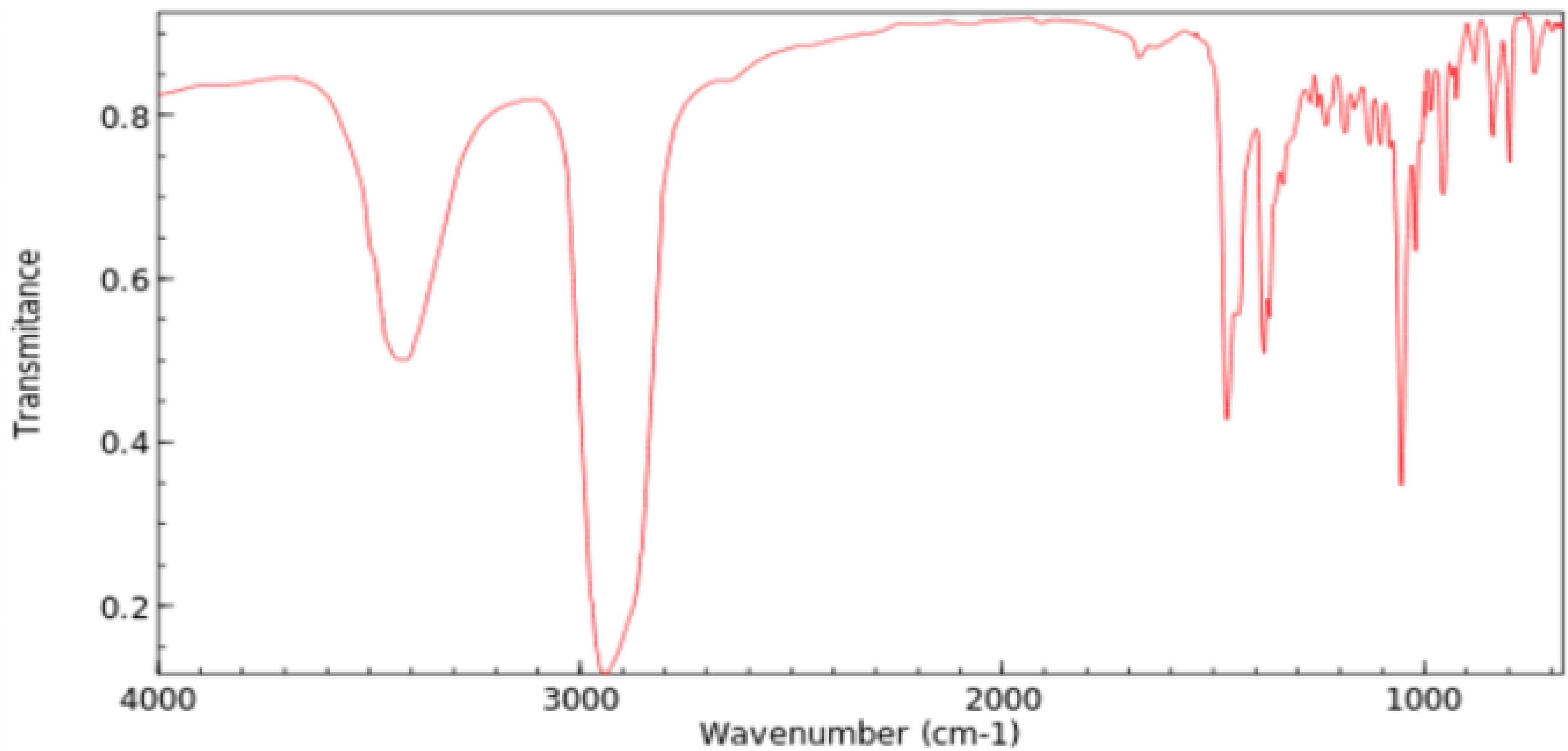


Bacterial ribosomes consist of three ribosomal RNA (rRNA) molecules (23S, 16S, and 5S) and more than 50 proteins (faded structures in this image). The rRNA molecules are divided between a large subunit and a small subunit. Transfer RNA (tRNA) brings amino acids to the ribosome, binding first to the aminoacyl (A) site, then the peptidyl (P) site, and finally the exit (E) site (not shown). This structure of an *Escherichia coli* ribosome was obtained with cryo-electron microscopy with 2 Å resolution.

Mass Spectrum—Cholesterol



IR Spectrum—Cholesterol



Publishing Chemistry—the Most Complex in STM

Composition Systems

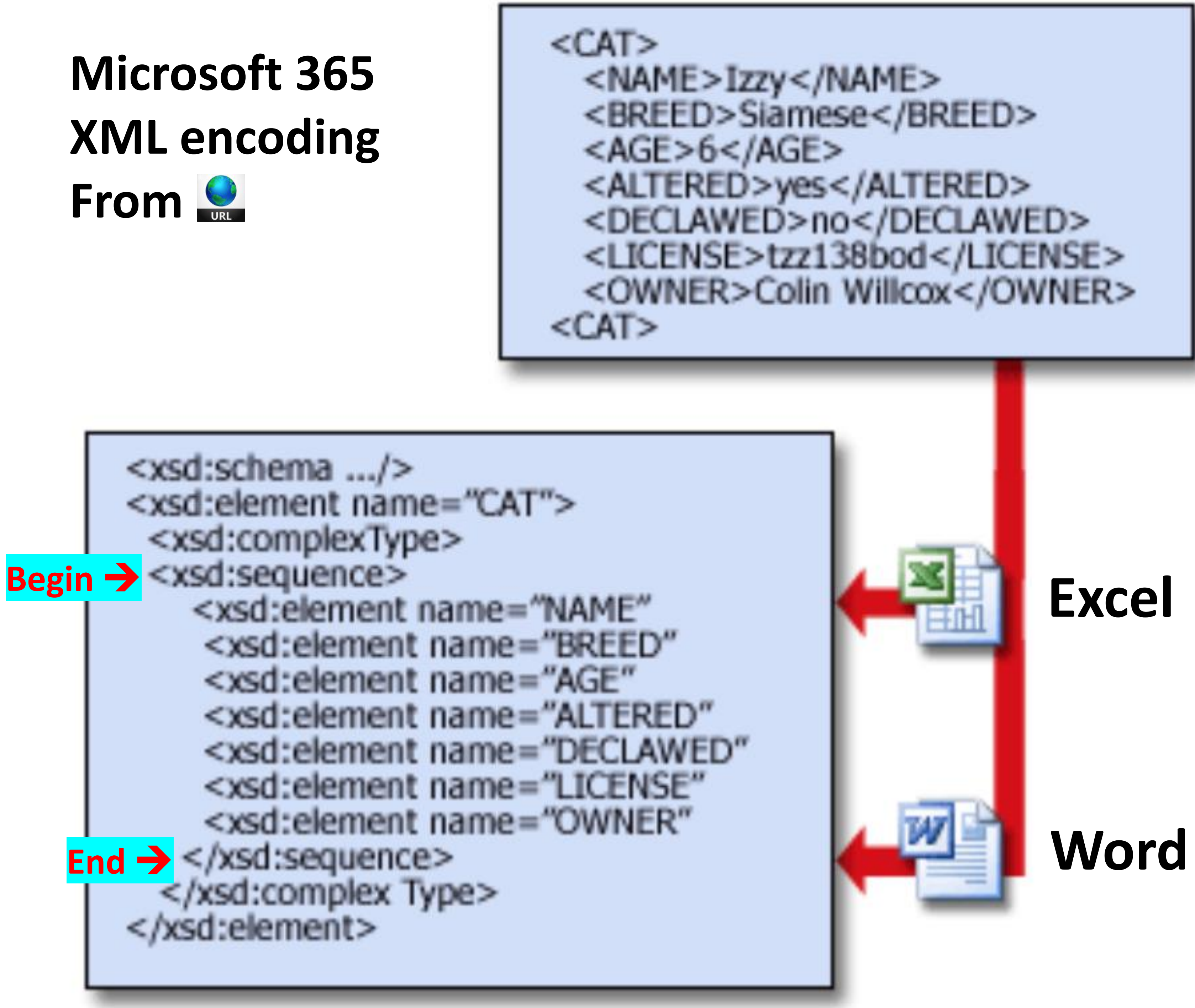
- Think Microsoft Word on steroids “Super Word”
  - ✓ adjust objects positions ± 0.001 in
  - ✓ create printing templates 4, 8, 16 pp/“sheet”
- Historically focus on traditional printing
  - ✓ Manuscripts → Printed pages in journal issues
- Modern composition systems also accommodate electronic publishing
  - ✓ Manuscripts → Printed pages [**and**] PDF, HTML, search fields, etc.

Internal Markup—XML

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE recipe PUBLIC "-//Happy-Monkey//DTD RecipeBook//EN"
"http://www.happy-monkey.net/recipebook/recipebook.dtd">

Begin → <recipe>

    Begin → <title>Peanut-butter On A Spoon</title> ← End

    Begin → <ingredientlist>
        Begin → <ingredient>Peanut-butter</ingredient> ← End
            </ingredientlist> ← End

    Begin → <preparation>
                Stick a spoon in a jar of peanut-butter,
                scoop and pull out a big glob of peanut-butter.
            </preparation> ← End

  End → </recipe>
```

For more information see URL URL

Microsoft 365
XML encoding
From



Evolution of Printing

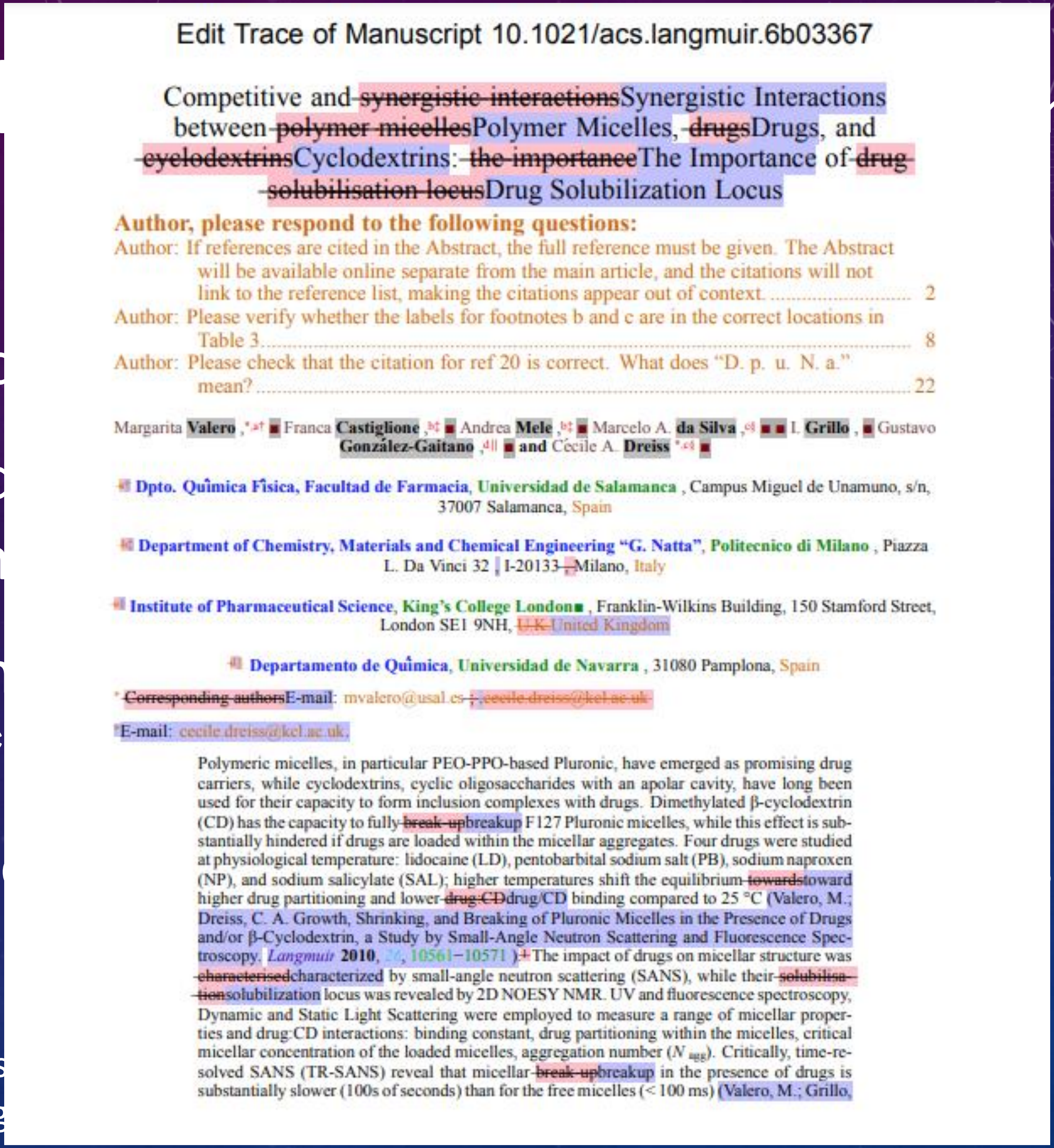
Woodblock printing	200
Movable type	1040
Printing press	c. 1440
Etching	c. 1515
Mezzotint	1642
Aquatint	1772
Lithography	1796
Chromolithography	1837
Rotary press	1843
Hectograph	1860
Offset printing	1875
Hot metal typesetting	1884
Mimeograph	1885
Photostat and rectigraph	1907
Screen printing	1911
Spirit duplicator	1923
Dot matrix printing	1925
Xerography	1938
Spark printing	1940
Phototypesetting	1949
Inkjet printing	1950
Dye-sublimation	1957
Laser printing	1969
Thermal printing	c. 1972
Solid ink printing	1972
3D printing	1986
Digital printing	1991

The Publishing Process

- Author creates manuscript and sends to journal scientific editor
- Scientific editor decides yes/no for consideration to publish—if yes…
- Scientific editor sends manuscript to 2-4 reviewers (experts in the specific area of investigation)—the <u>peer</u> <u>review</u> process
- Reviewer ⇆ Scientific editor ⇆ Author revises manuscript based on reviewers' comments

Th… nt.)

- The … or send…
- Prod… man…
- Man… file*
- Tabl… , etc.



Edit Trace of Manuscript 10.1021/acs.langmuir.6b03367

Competitive and ~~synergistic interactions~~Synergistic Interactions between ~~polymer micelles~~Polymer Micelles, ~~drugs~~Drugs, and ~~cyclodextrins~~Cyclodextrins: ~~the importance~~The Importance of ~~drug solubilisation locus~~Drug Solubilization Locus

Author, please respond to the following questions:

Author: If references are cited in the Abstract, the full reference must be given. The Abstract will be available online separate from the main article, and the citations will not link to the reference list, making the citations appear out of context. 2

Author: Please verify whether the labels for footnotes b and c are in the correct locations in Table 3. 8

Author: Please check that the citation for ref 20 is correct. What does "D. p. u. N. a." mean? 22

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Polymeric micelles, in particular PEO-PPO-based Pluronic, have emerged as promising drug carriers, while cyclodextrins, cyclic oligosaccharides with an apolar cavity, have long been used for their capacity to form inclusion complexes with drugs. Dimethylated β-cyclodextrin (CD) has the capacity to fully ~~break-up~~breakup F127 Pluronic micelles, while this effect is substantially hindered if drugs are loaded within the micellar aggregates. Four drugs were studied at physiological temperature: lidocaine (LD), pentobarbital sodium salt (PB), sodium naproxen (NP), and sodium salicylate (SAL); higher temperatures shift the equilibrium ~~towards~~toward higher drug partitioning and lower ~~drug:CD~~drug/CD binding compared to 25 °C (Valero, M.; Dreiss, C. A. Growth, Shrinking, and Breaking of Pluronic Micelles in the Presence of Drugs and/or β-Cyclodextrin, a Study by Small-Angle Neutron Scattering and Fluorescence Spectroscopy. *Langmuir* **2010**, *26*, 10561−10571) ~~+~~ The impact of drugs on micellar structure was ~~characterised~~characterized by small-angle neutron scattering (SANS), while their ~~solubilisation~~solubilization locus was revealed by 2D NOESY NMR. UV and fluorescence spectroscopy, Dynamic and Static Light Scattering were employed to measure a range of micellar properties and drug:CD interactions: binding constant, drug partitioning within the micelles, critical micellar concentration of the loaded micelles, aggregation number (N_{agg}). Critically, time-resolved SANS (TR-SANS) reveal that micellar ~~break-up~~breakup in the presence of drugs is substantially slower (100s of seconds) than for the free micelles (< 100 ms) (Valero, M.; Grillo,

* Micros… packag…

The Publishing Process (cont.)

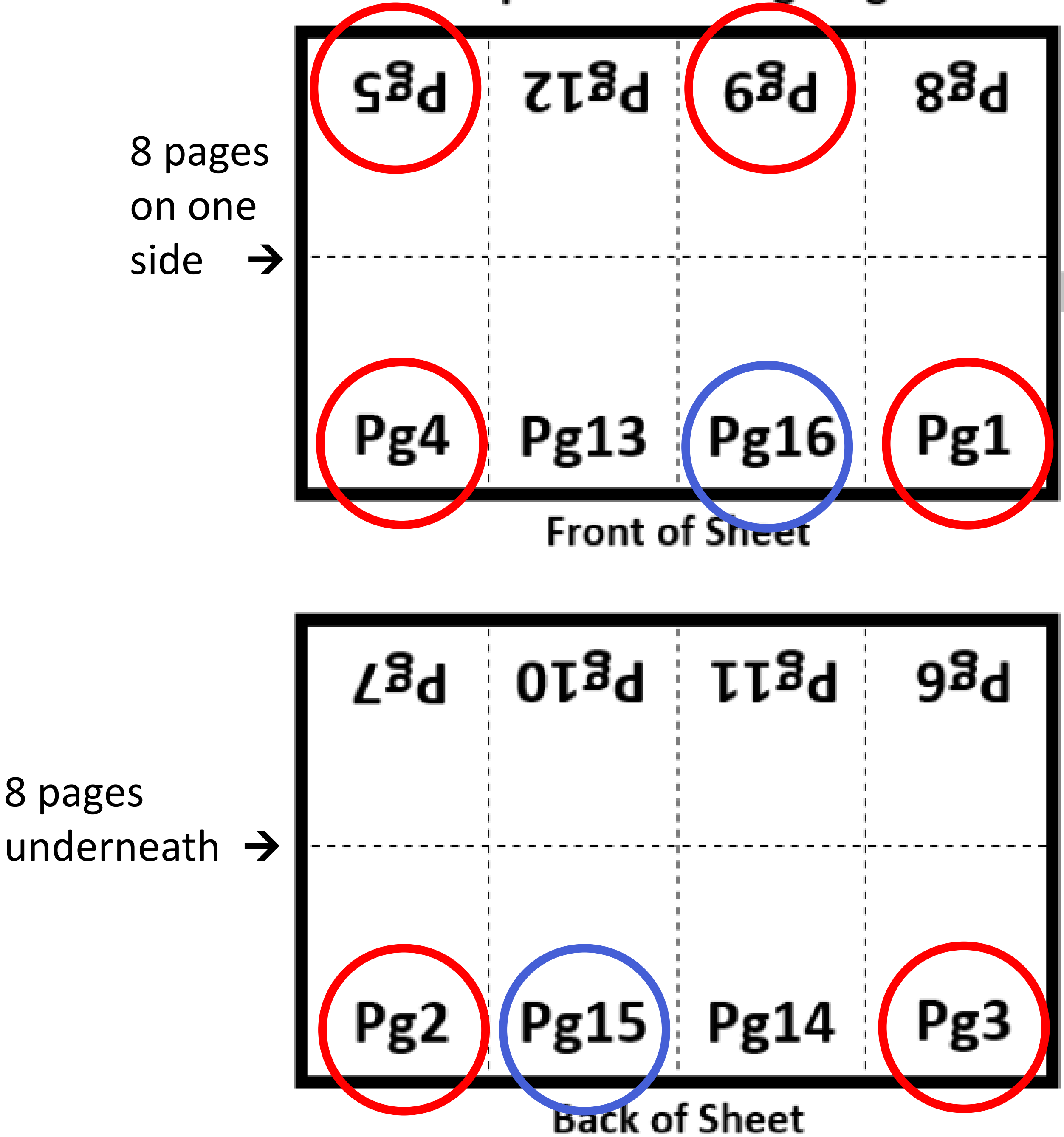
- Article proof created
  - ✓ checked by production editor
  - ✓ sent to author
- Author returns corrected proof to production editor
- Article assigned to an issue and placement
- The issue is prepared for printing through composition system

Creation of Printed Journal

- From the composition system—forms are prepared for printing…
  - ✓ for 4-up, 8-up, 16-up printing (signatures)
- Issue printed
- Pages trimmed and bound
- Issue mailed


BHS
SP-X

An Example of a 16-Page Signature



Signatures are folded, trimmed and bound to make the issue

Electronic Version Preparation

- Processing done on an article-by-article basis from the composition system
  - ✓ Indexing elements extracted from composition system (title, author, affiliation, year, abstract, text, etc.)
  - ✓ PDF file created
  - ✓ HTML file created
  - ✓ Index created from extracted elements
- Article loaded in RDBMS, server, etc.

The challenges on the road to electronic publishing?

How Long for Development?

- My first estimate in 1974—2 to 3 years
- On second thought in 1975—4, 5, maybe 6 years
- Oh so naïve—it took 28 years!

Challenges to Electronic Publishing

- Many technical Issues
- Requirement for print **and** electronic journals
- Differing philosophies among stakeholders…
  - ✓ "Electronic is the wave of the future"
  - ✓ "If it ain't broke don't fix it" "Paper forever!"
- Internal fiefdoms and power struggles
- Competition for resources (R&D is expensive)

Ah… … the Technical Challenges

Availability of Computers

- 1974—no PCs or Apple computers, no iPads
  - ✓ 1970—a IBM System 370 introduced
  - ✓ 1975—Microsoft established
  - ✓ 1976—Apple founded
  - ✓ 1970s—Apple I & II, TRS-80, Commodore
  - ✓ 1980s—IBM PC, Dell, HP, Apple (labs and libraries)
- In 1980s computers still not ubiquitous

Telecommunications

- 1980—Communications over phone lines* at 300 baud= 300 bits/sec = 0.0003 Mbps
  - ✓ *ACR* article 121 KB (PDF)—requires 53 min 47 sec to download
  - ✓ 3.5 MB photo (JPEG)—requires 25.93 hours to download

* Using an acoustic coupler

Telecommunications (cont.)

- 1984—ACS established T1 lines: Columbus, OH to Tokyo, Japan and Karlsruhe, Germany—1.544 Mbps
  - ✓ *ACR* article 121 KB (PDF)—requires 0.627 sec to download
  - ✓ 3.5 MB photo (JPEG)—requires 18.1 sec to download
- T1 shared among numerous tasks and very expensive

Telecommunications (cont.)

- **Today**—My house: 300 Mbps down and 340 Mbps up* (equal to ~200 T1 lines or ~7 T3 lines)
  - ✓ *ACR* article 121 KB (PDF)—requires 0.00323 seconds to download
  - ✓ 3.5 MB photo (JPEG)—requires 0.093 seconds to download

* Verizon FiOS

Cost of Data Storage

- 1974—75 MB hard disk drive
  - ✓ $12,500 ($44,600 in 2021 dollars)
  - ✓ $594,000/TB
- 2021—4 TB Hitachi disk drive
  - ✓ $70
  - ✓ $17.50/TB

Cooperative Experiments

- 1989-1995: CORE project to build a prototype digital library at Cornell University
  - ✓ ACS, Belcore, Chemical Abstracts Service, Cornell University and Ohio Computer Library Center (OCLC)
- 1992-1997: Red Sage Project another prototype digital library
  - ✓ 20 publishers with UC-San Francisco
- Efforts made obsolete by WWW & Internet

ACS Highlights for Electronic Publishing

- 1980—1,000 articles from *J. Med. Chem*. on BRS* (text only)
- 1982—all 16 ACS journals on BRS** (text only)
- 1996—*J. Phys. Chem*. (100th anniversary) on STN International

* Bibliographic Retrieval Services. Today sold as LiveLink ECM Discovery Server by Open Text Corporation

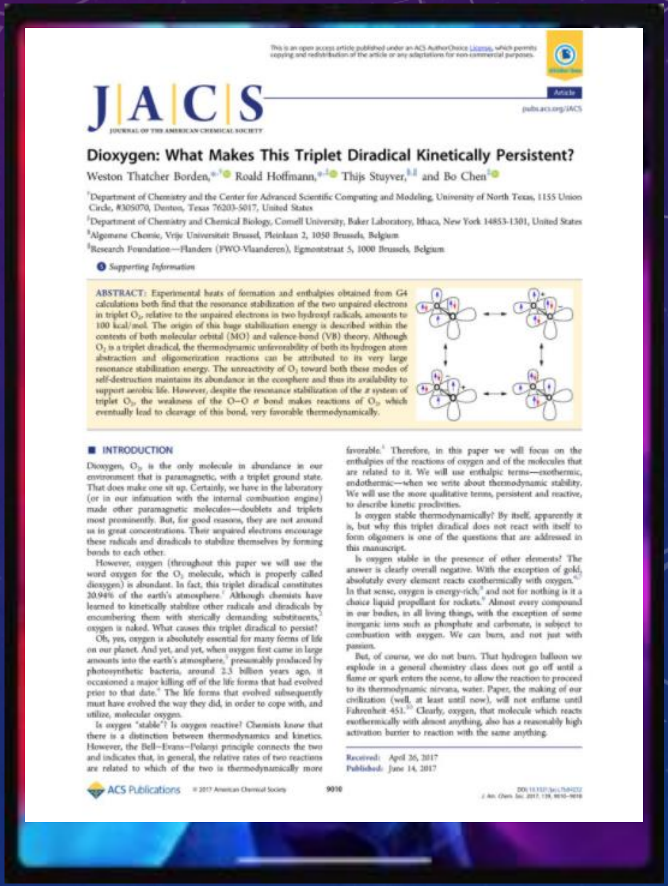
** 1974-1980, goal achieved after 8 years?

Timeline for Electronic Publishing (cont.)

- 1997—presentation to ACS Board of Directors then scientists at ACS National Meeting in Las Vegas
- 1997—all 26 ACS journals on STN International
- 2002—all ACS journals, from 1879 forward, on STN International (graphics, math, tables, chemical structures, etc.)

- 1974 to 2002—28 years!

Thanks for your attention!



JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Article
pubs.acs.org/JACS

Dioxygen: What Makes This Triplet Diradical Kinetically Persistent?

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Supporting Information

ABSTRACT: Experimental heats of formation and enthalpies obtained from G4 calculations both find that the resonance stabilization of the two unpaired electrons in triplet O_2, relative to the unpaired electrons in two hydroxyl radicals, amounts to 100 kcal/mol. The origin of this huge stabilization energy is described within the contexts of both molecular orbital (MO) and valence-bond (VB) theory. Although O_2 is a triplet diradical, the thermodynamic unfavorability of both its hydrogen atom abstraction and oligomerization reactions can be attributed to its very large resonance stabilization energy. The unreactivity of O_2 toward both these modes of self-destruction maintains its abundance in the ecosphere and thus its availability to support aerobic life. However, despite the resonance stabilization of the π system of triplet O_2, the weakness of the O–O σ bond makes reactions of O_2, which eventually lead to cleavage of this bond, very favorable thermodynamically.

INTRODUCTION

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