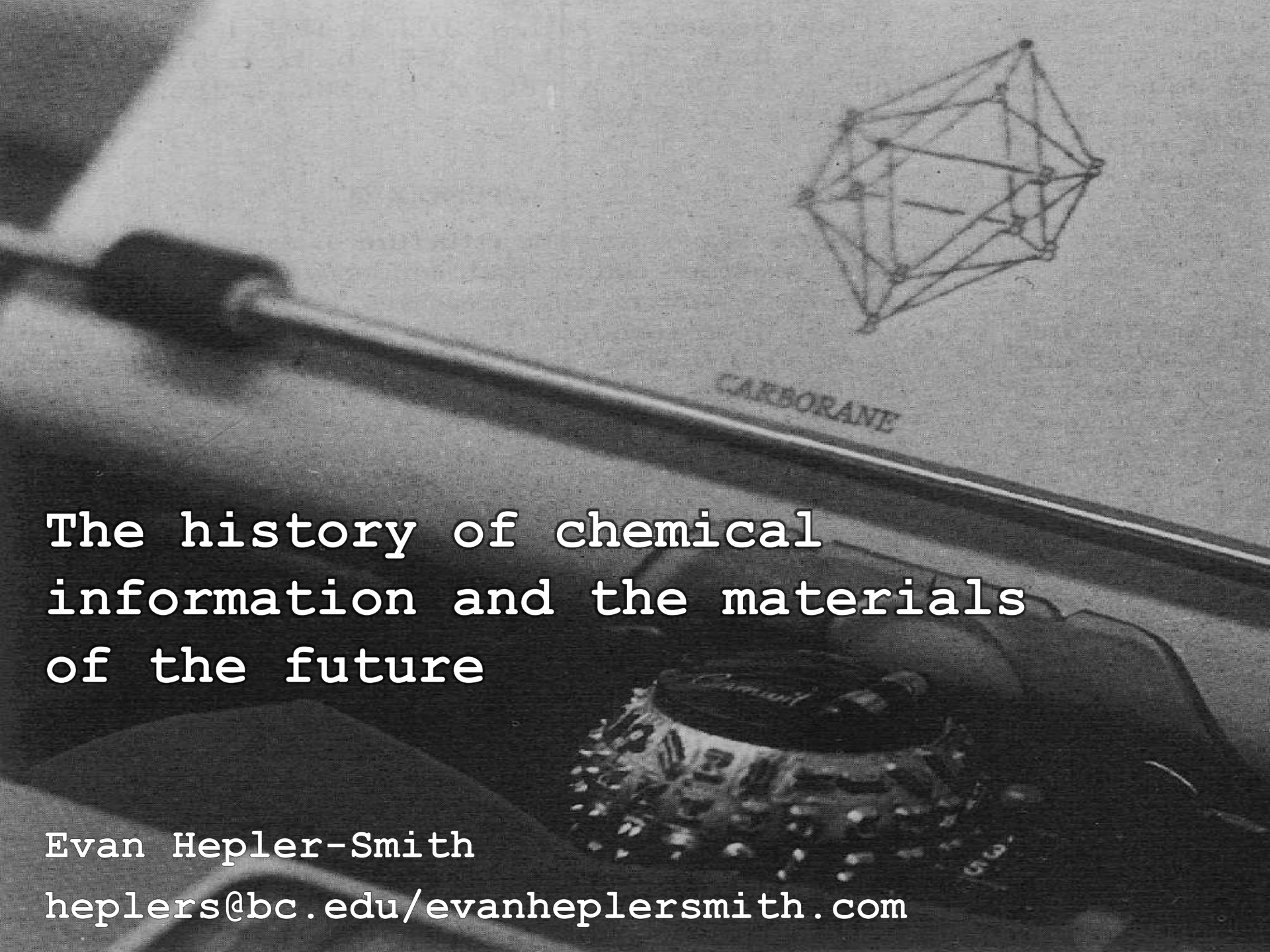
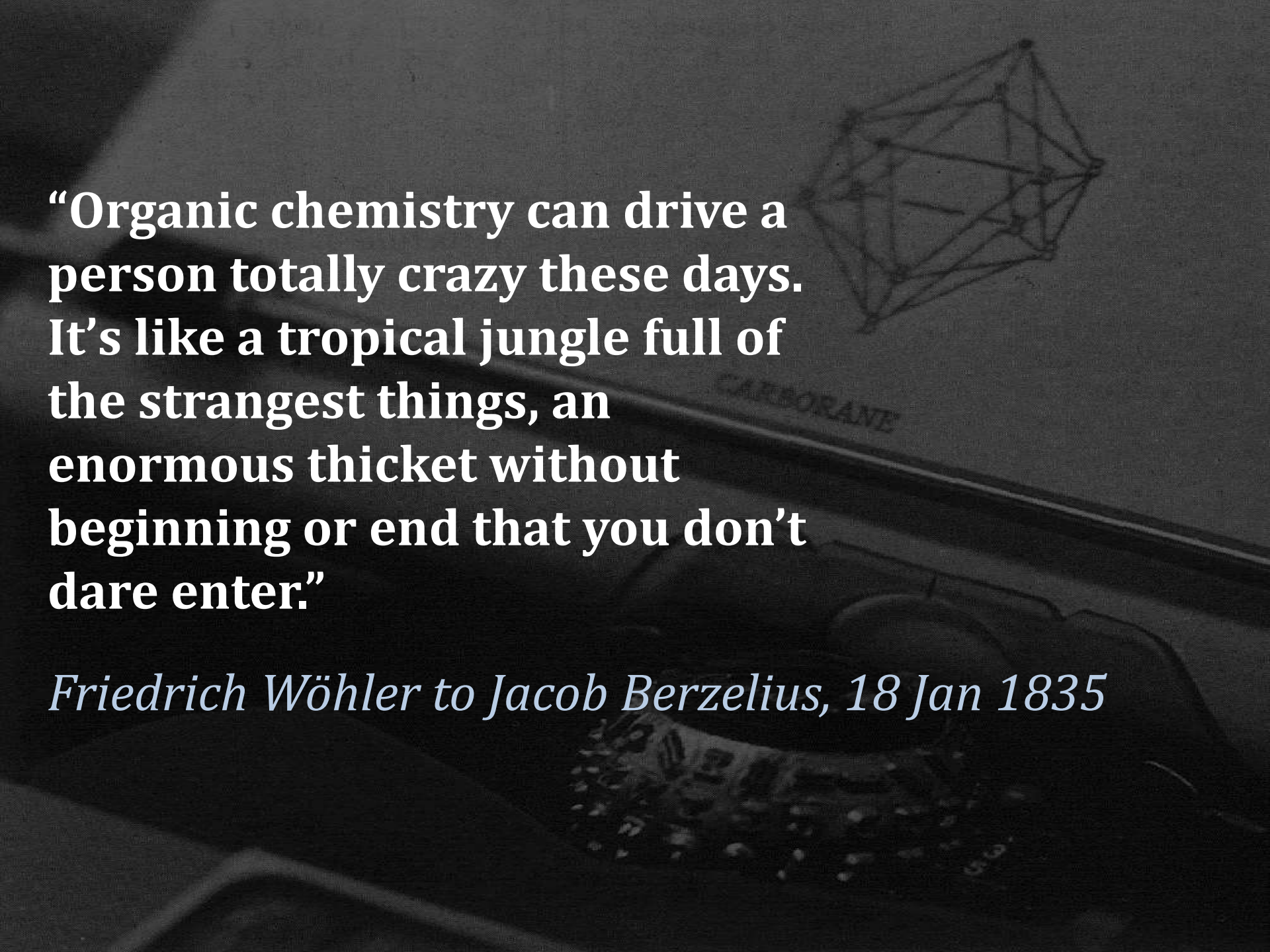


The history of chemical information and the materials of the future

Evan Hepler-Smith
heplers@bc.edu/evanheplersmith.com



“Organic chemistry can drive a person totally crazy these days. It’s like a tropical jungle full of the strangest things, an enormous thicket without beginning or end that you don’t dare enter.”

Friedrich Wöhler to Jacob Berzelius, 18 Jan 1835

“It’s like a tropical jungle full of the strangest things, an enormous thicket without beginning or end that you don’t dare enter.”

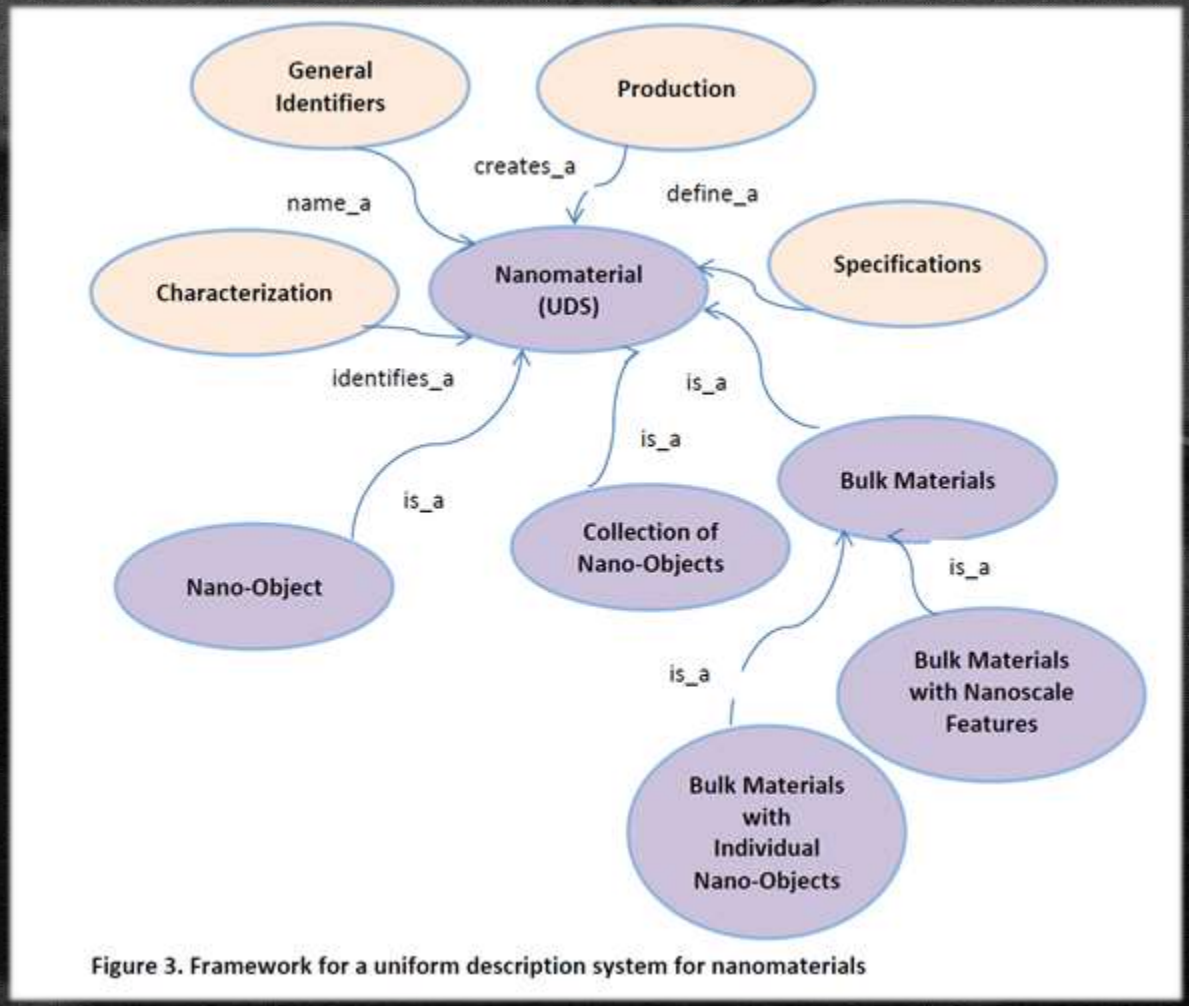
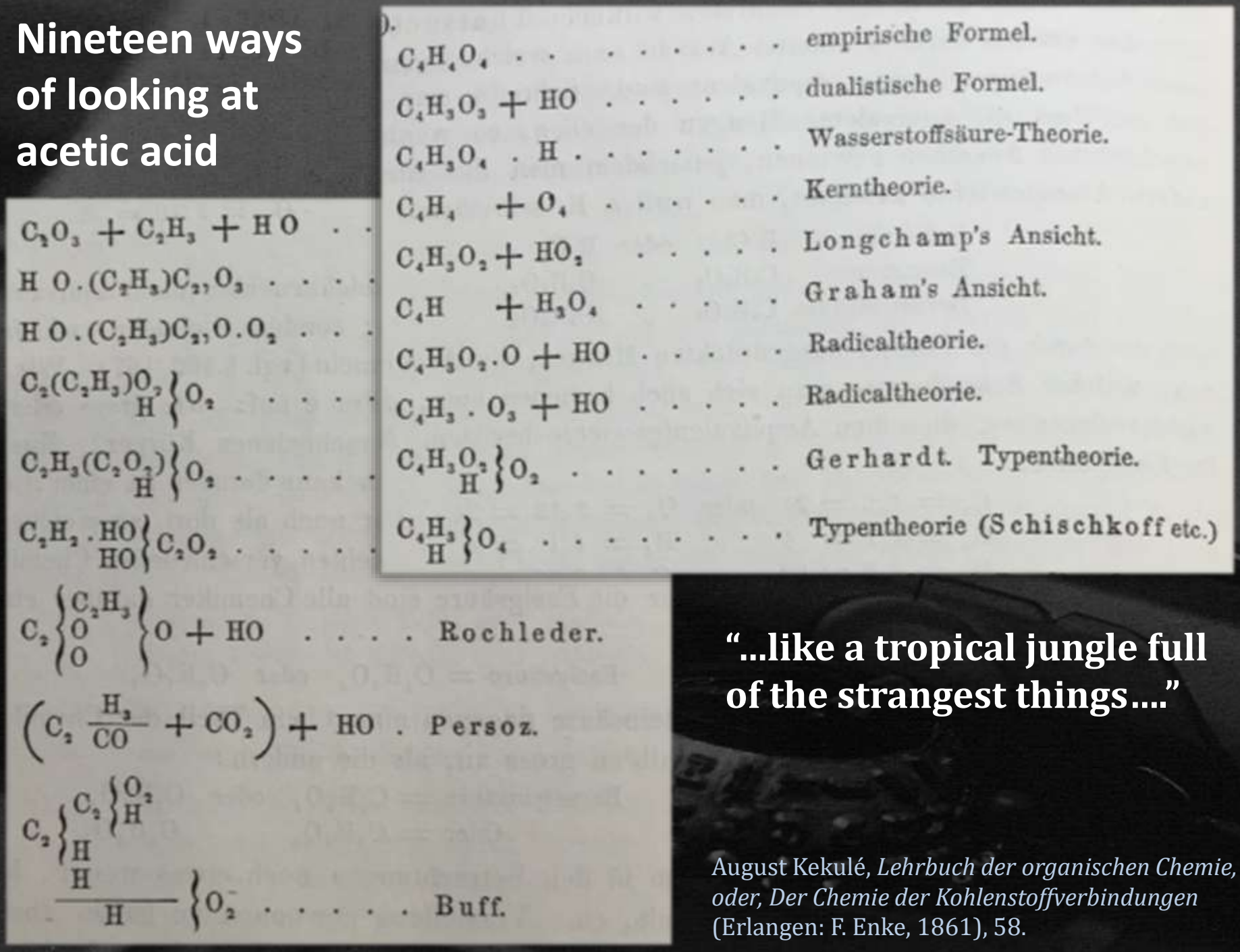


Figure 3. Framework for a uniform description system for nanomaterials

CODATA-VAMAS Working Group On the Description of Nanomaterials, “Uniform Description System for Materials on the Nanoscale, Version 2.0” (June 30, 2016), https://doi.org/10.5281/zenodo.56720, 14.

Nineteen ways of looking at acetic acid



$C_4H_4O_4$ . . . . . empirische Formel.

$C_4H_3O_3 + HO$ . . . . . dualistische Formel.

$C_4H_3O_4 . H$ . . . . . Wasserstoffsäure-Theorie.

$C_4H_4 + O_4$ . . . . . Kerntheorie.

$C_4H_3O_2 + HO_2$ . . . . . Longchamp's Ansicht.

$C_4H + H_3O_4$ . . . . . Graham's Ansicht.

$C_4H_3O_2.O + HO$ . . . . . Radicaltheorie.

$C_4H_3 . O_3 + HO$ . . . . . Radicaltheorie.

$C_4H_3O_2\}O_2$ . . . . . Gerhardt. Typentheorie.

$C_4H_3\}O_4$ . . . . . Typentheorie (Schischkoff etc.)

$C_2O_3 + C_2H_3 + HO$ . .

$HO.(C_2H_3)C_2O_3$ . . . .

$HO.(C_2H_3)C_2O.O_2$ . . .

$C_2(C_2H_3)O_2\}O_2$ . . . .

$C_2H_3(C_2O_2)\}O_2$ . . . . .

$C_2H_2.HO\}C_2O_2$ . . . . .

$C_2\{C_2H_3\}O + HO$ . . . . Rochleder.

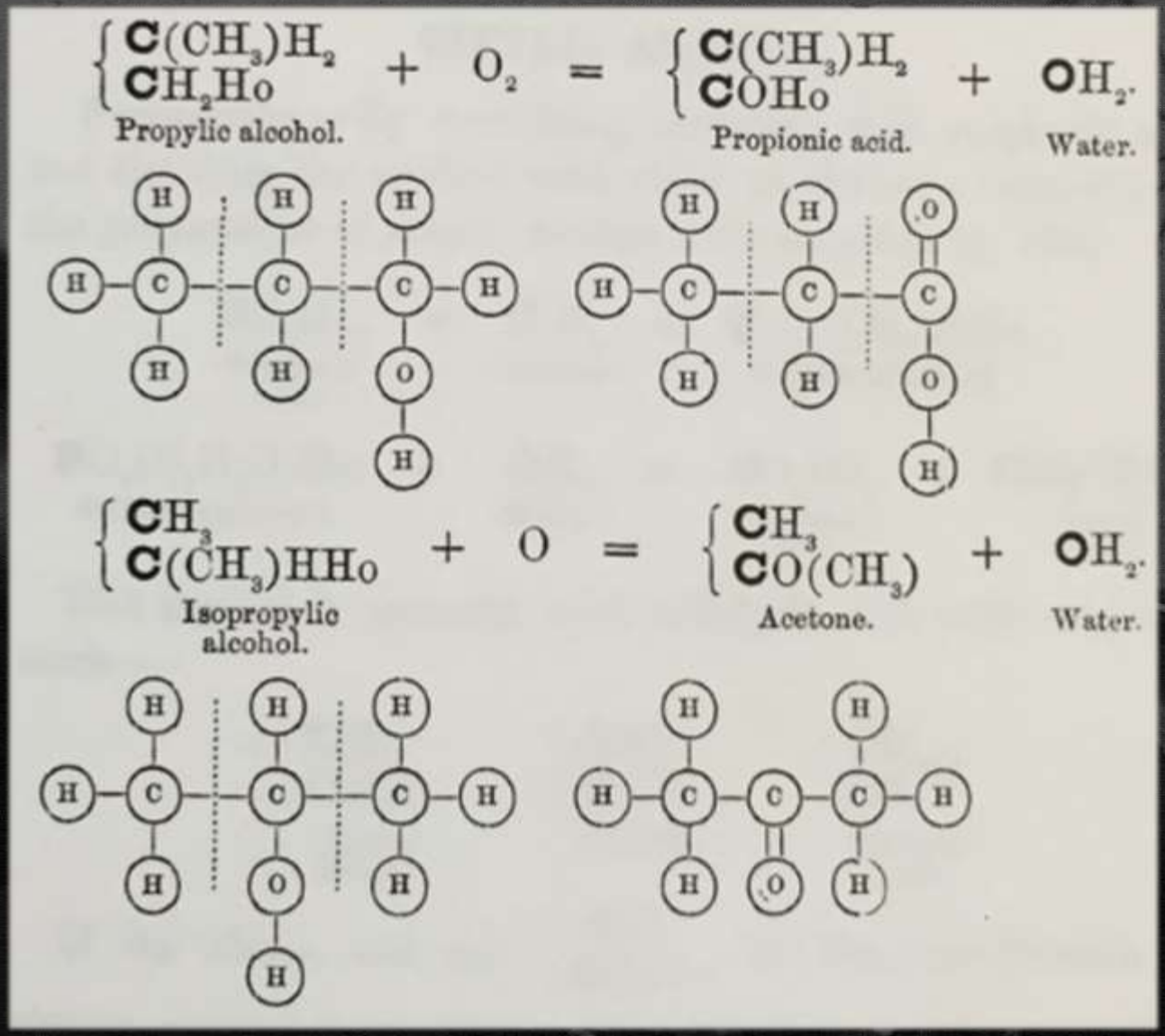
$\left(C_2\frac{H_3}{CO} + CO_2\right) + HO$. Persoz.

$C_2\{C_2\{O_2\}H\}H$

$\frac{H}{H}\}O_2$ . . . . . Buff.

"...like a tropical jungle full of the strangest things...."

August Kekulé, *Lehrbuch der organischen Chemie, oder, Der Chemie der Kohlenstoffverbindungen* (Erlangen: F. Enke, 1861), 58.



Edward Frankland, *Lecture Notes for Chemical Students* (1866), adopting the notation of Alexander Crum Brown

HOW MACHINE LEARNING AND BIG DATA ARE HELPING CHEMISTS SEARCH THE VAST CHEMICAL UNIVERSE FOR BETTER MEDICINES.

THE DRUG-MAKER'S GUIDE TO THE GALAXY

"The team can comb through all 166 billion compounds in the database for compelling candidates…The approach is like using a geological map to work out where to dig for gold…or to pan lots of locations for gold without worrying too much about the starting location…"

"The bottleneck in our exploration of chemical space is the ability to dare to make compounds." (2017)

THE DRUG-MAKER'S GUIDE TO THE GALAXY

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"The bottleneck in our exploration of chemical space is the ability to dare to make compounds." (2017)

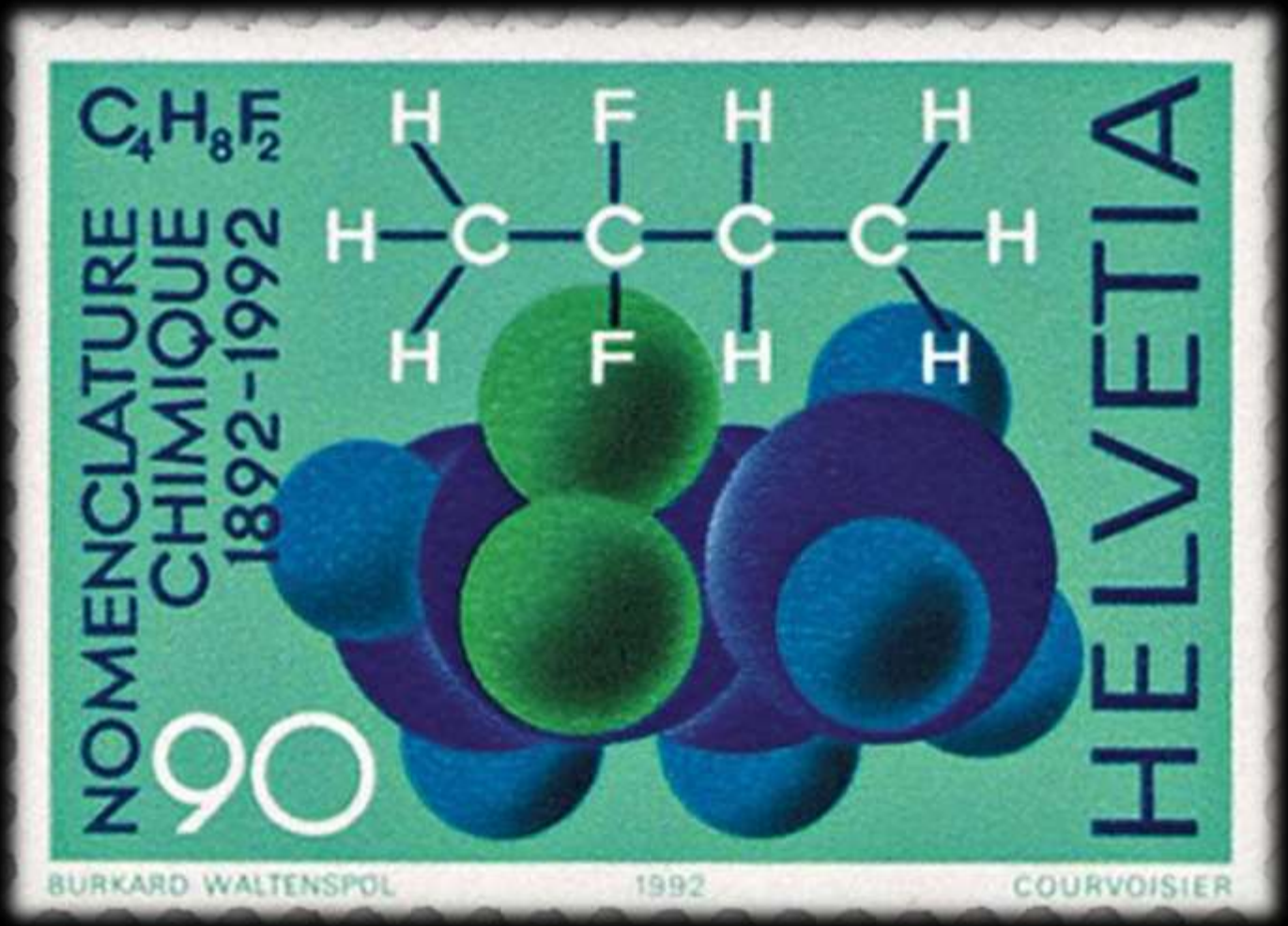
"The material science of chemistry is becoming a third-order science of information." 1969!

"Among all of the chemist's instruments, none is more indispensable than good information resources. A chemist can no more do without these than without the balance or the thermometer." 1919!

"As in a gold rush, researchers in organic chemistry push single-mindedly toward the goal of striking gold…. Given the seemingly inexhaustible wealth of the land, the work inevitably becomes somewhat mechanical." 1887!

Compound Words

Chemists, Information, and the Synthetic World



Plan for today

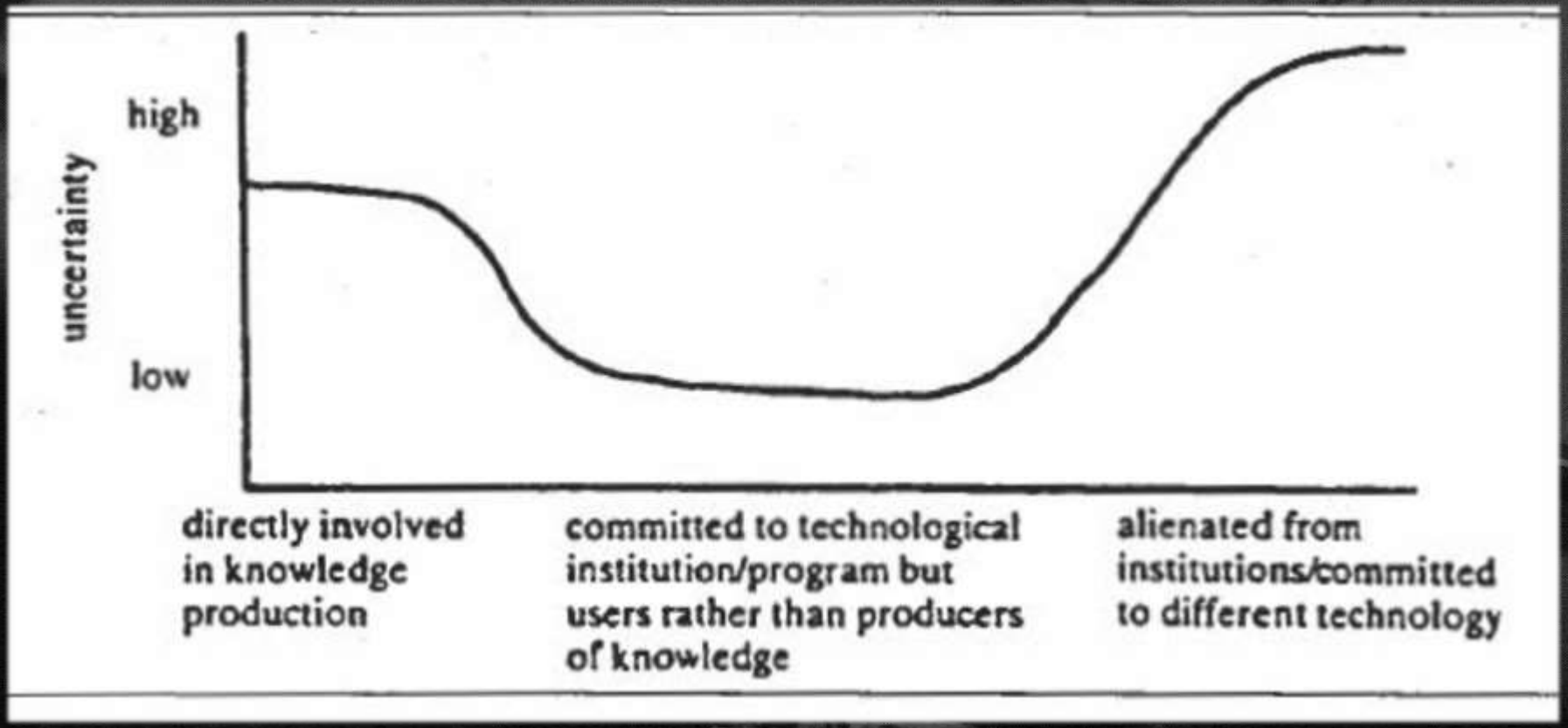
1. A little social science jargon

2. Where systematic nomenclature came from

3. How chemical information got database'd

4. Molecular bureaucracy

"The Certainty Trough"



Sociologist Donald Mackenzie, writing about who is certain & uncertain about nuclear missile accuracy, 1990

Ontological pluralism: roads (mostly) not taken as alternatives to molecular structure

"Instead of hypothesizing about molecular structure, I define substances by their metamorphoses, that is, by their past and by their future."

Alsatian-French chemist Charles Gerhardt, 1850

[N]ew concepts such as "ordered structure," "real or dummy ordered substructure", "hyperstructure", which meet the requirements of computer-based modern chemistry.

Jacques-Émile Dubois (DARC system creator), 1974

Ontological pluralism

"The simplification of ontology has led to the enormous complication of epistemology."

Anthropologist Eduardo Vivieros de Castro, 2004 (describing the struggles of Western anthropologists to understand cosmologies and kinship among animist Amerindian cultures in South America… but doesn't this nicely describe efforts to do environmental toxicology, policy, and politics on a molecule by molecule basis?)

Ontological pluralism

“[T]he general picture of chemistry after the grand synthesis of organic structural theory is not one of a perfect unified science living happily ever after, but another pluralistic configuration of multiple imperfect systems competing and interacting with each other.”

Philosopher Hasok Chang, 2012

Enactment

For practical purposes, stuff doesn't just *exist* in some abstract, absolute way. Rather, an object is brought into existence and kept there—"enacted"—through activities, instruments, databases, and the ways that people and other objects relate to it. This means that sometimes the same stuff can be enacted as multiple objects at the same time.

EHS gloss on philosopher Annemarie Mol, The Body Multiple*, 2002. Mol's topic (disease) is particularly apt—but this goes for chemicals, too!*

United States Environmental Assessment Center

DHMO.org

Dihydrogen Monoxide Research Division

FAQs

Dihydrogen Monoxide FAQ

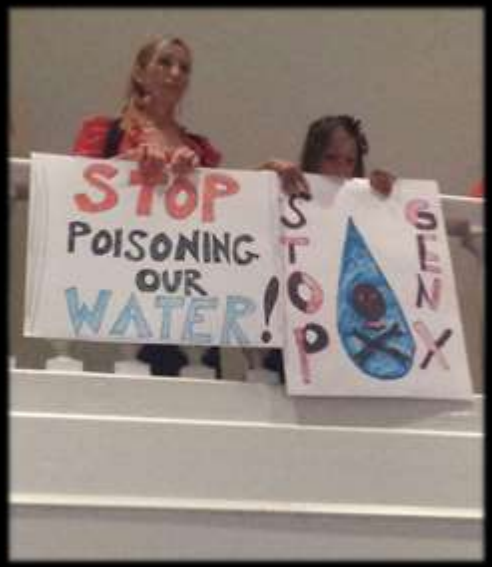
Frequently Asked Questions About Dihydrogen Monoxide (DHMO)

What is Dihydrogen Monoxide?

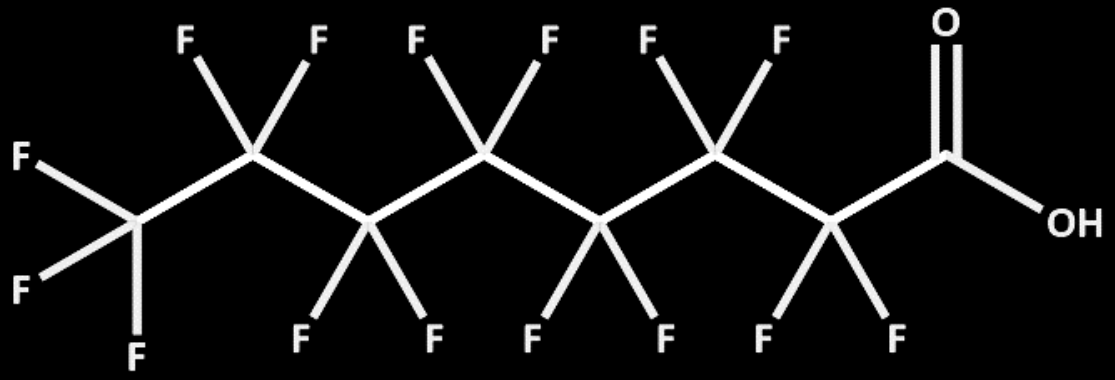
Dihydrogen Monoxide (DHMO) is a colorless and odorless chemical compound, also referred to by some as Dihydrogen Oxide, Hydrogen Hydroxide, Hydronium Hydroxide, or simply Hydric acid. Its basis is the highly reactive hydroxyl

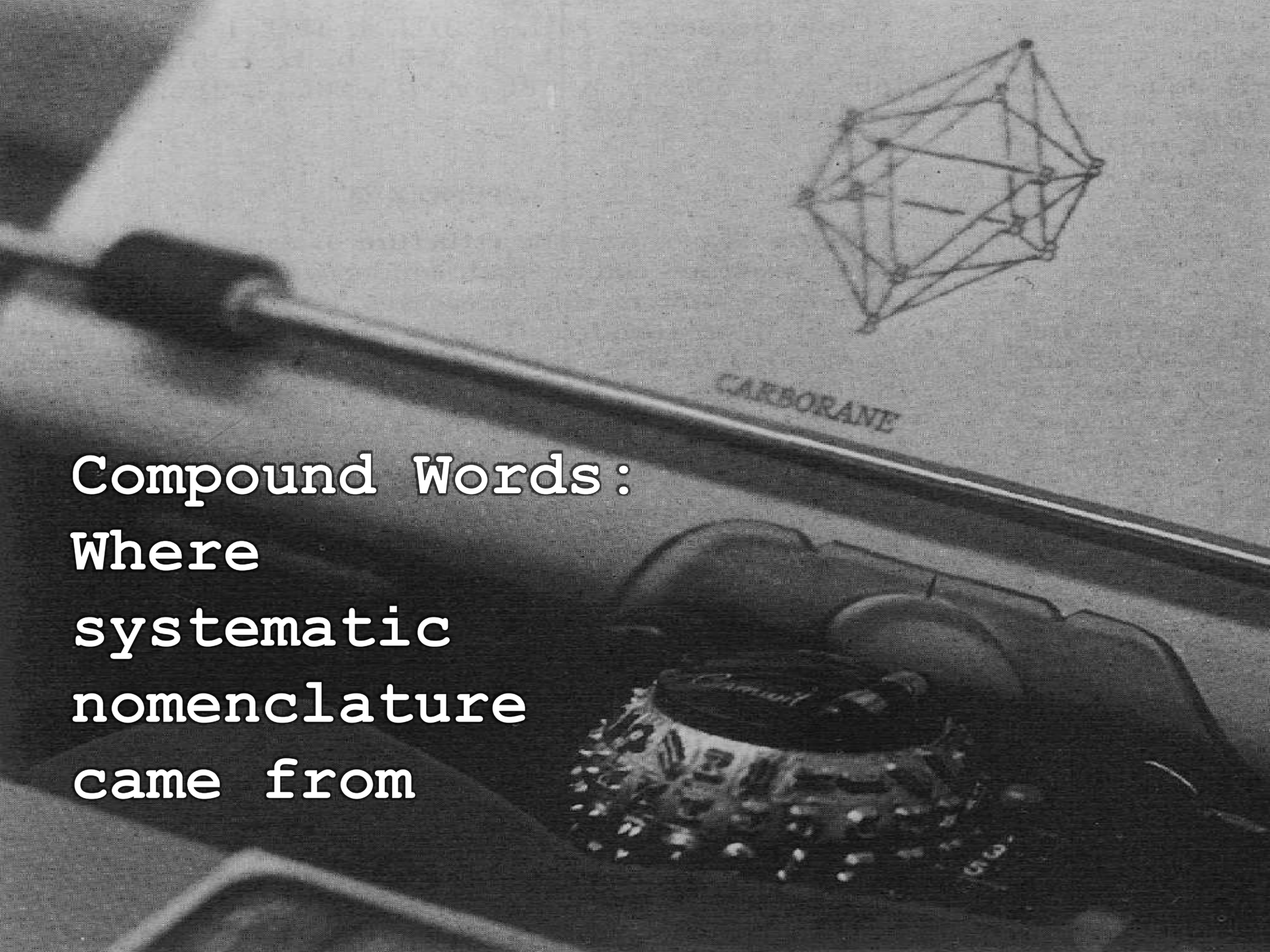
New Teflon Toxin Found in North Carolina Drinking Water
The Intercept - Jun 17, 2017

Environmental toxicologists: Fluorine-packed chemicals "as a whole, much more than solely PFOA, are an intractable, potentially never-ending chemicals management issue."

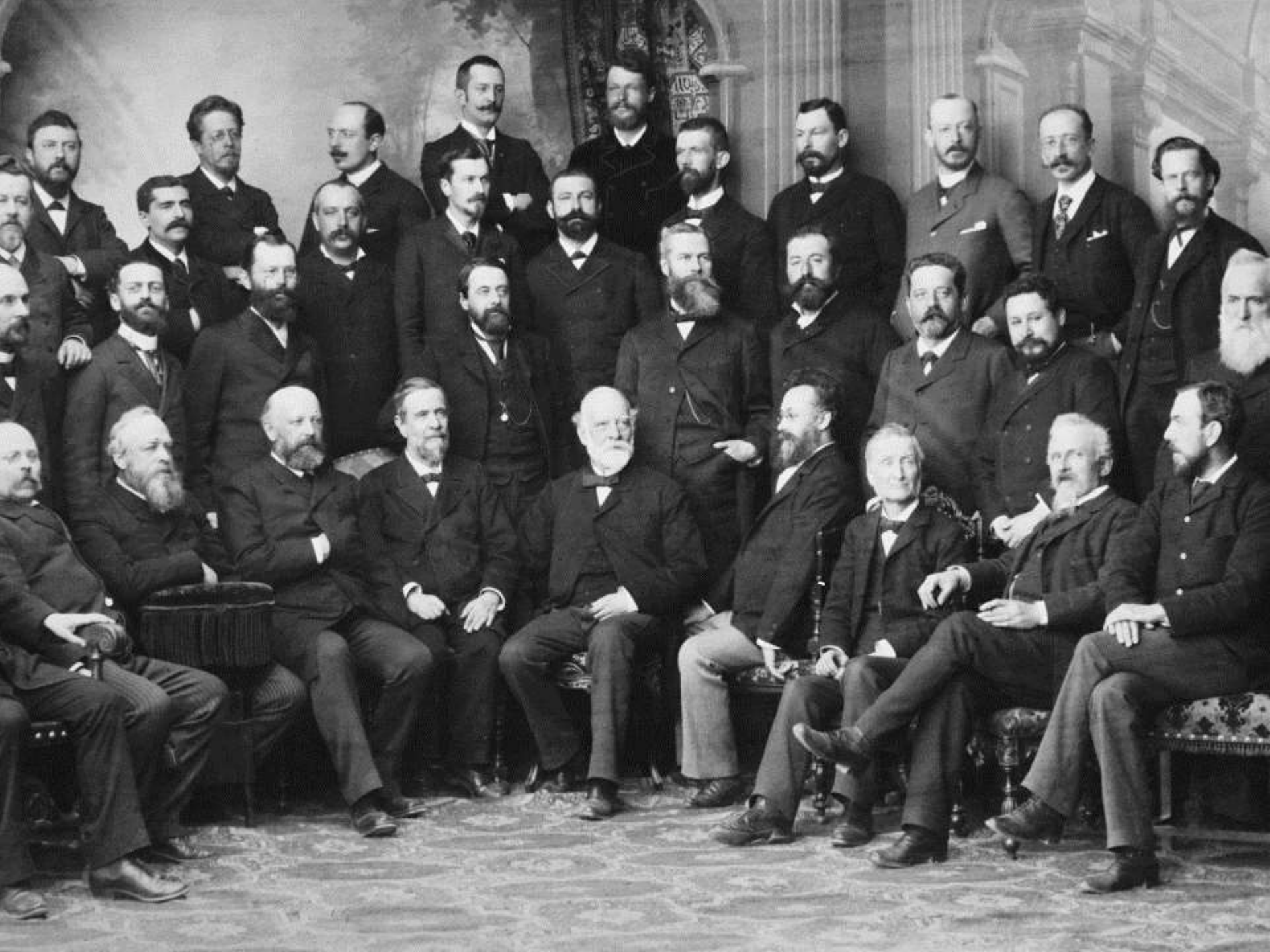


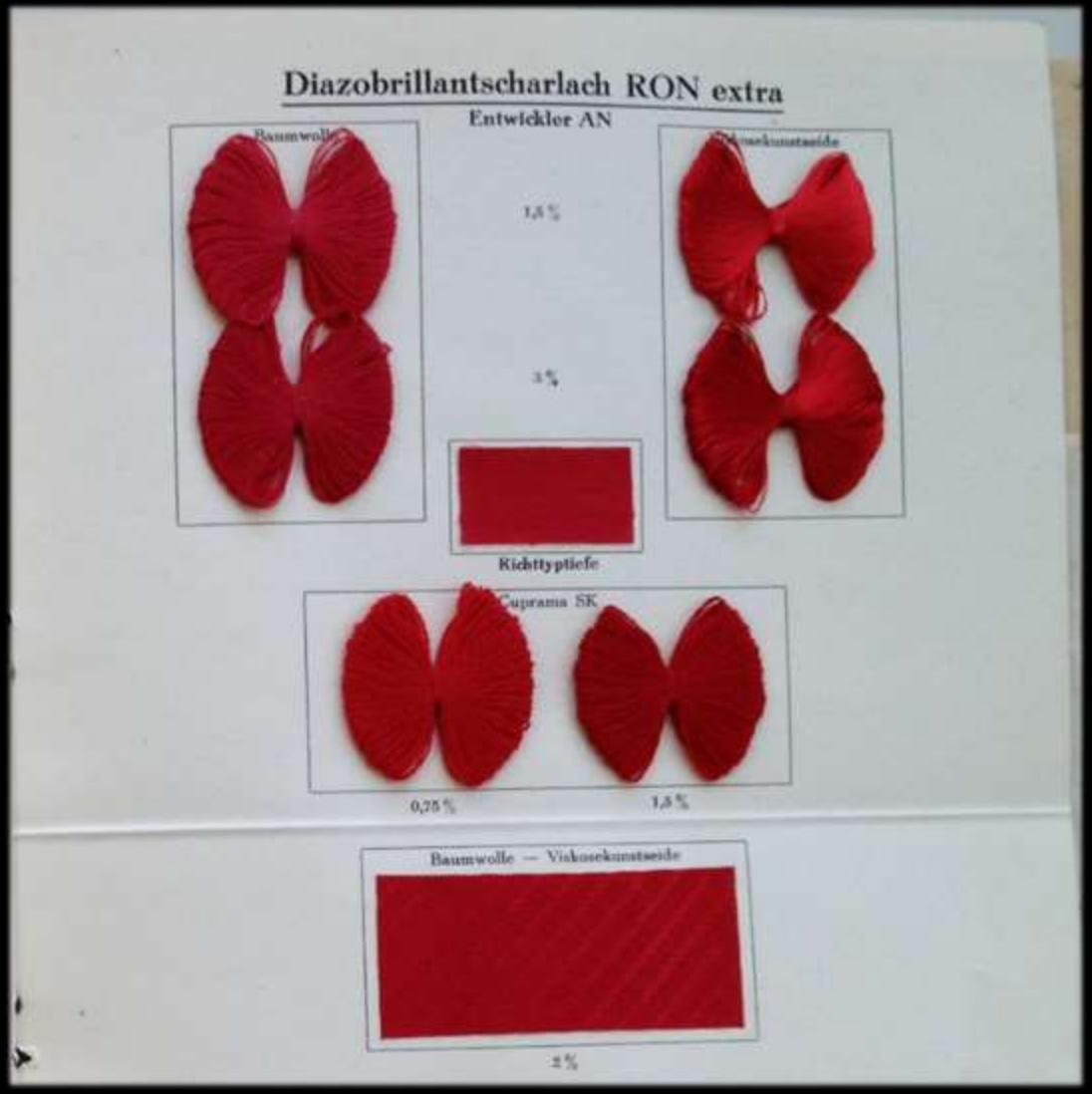
PFOA





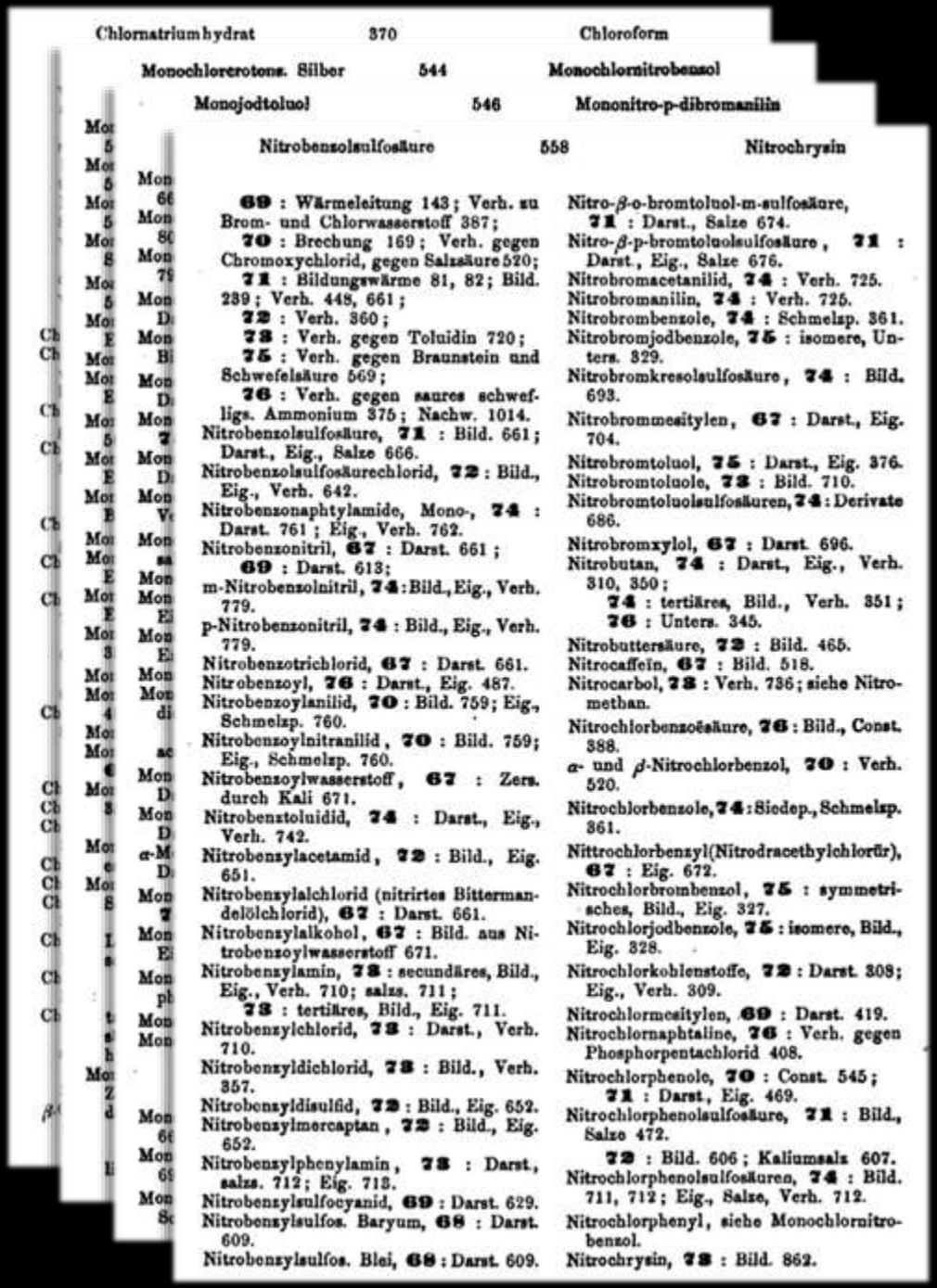
Compound Words:
Where
systematic
nomenclature
came from





“Diazo Brilliant Scarlet RON extra”
Bayer coal-tar dye samples

Catalog of Bayer drugs available in the US, circa 1905



Page 370:

Chlornitrobenzol, **71** : Bildungswärme 81; Verh. 431;
72 : Verh. 669, 670, 671;
74 : Darst. Eig. 372.
Chlornitrobenzol, **68** : α, Darst. 343.
Chlornitrobenzol, **68** : β, Darst. 344.

Page 544:

α- und β-Nitrochlorbenzol, **70** : Verh. 520.
Nitrochlorbenzole, **74** : Siedep., Schmelzp. 361.

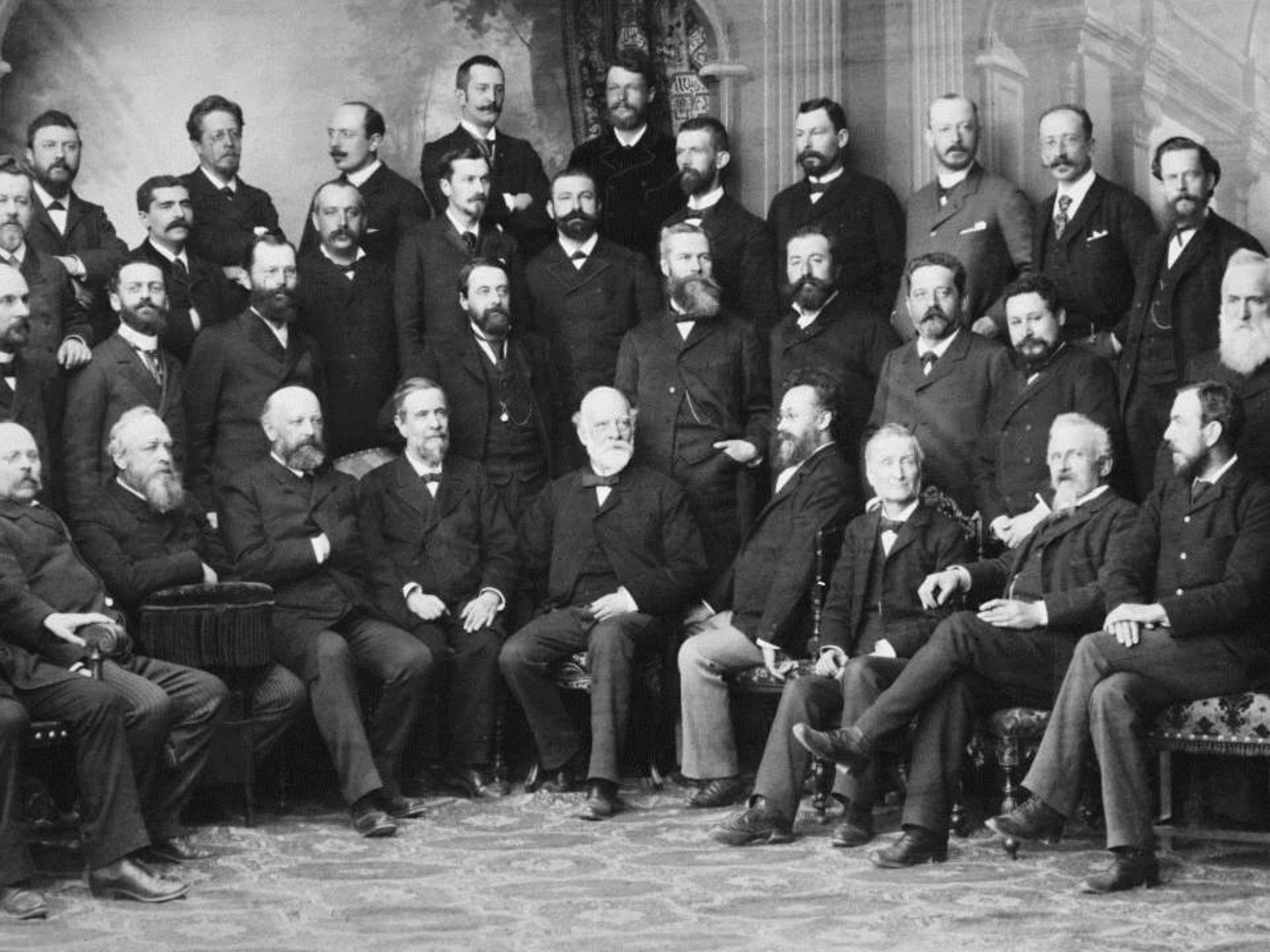
Page 546:

Monochlornitrobenzol (Nitrochlorphenyl), **67** : Bild. 631.

Page 558:

Mononitrochlorbenzol, **75** : Verh. 427.

Jahresbericht über die Fortschritte der Chemie und verwandter Theile anderer Wissenschaften, Register zu den Berichten, 1867-1876 (Giessen: J. Ricker, 1880).



RÉSOLUTIONS

PRISES PAR LA

COMMISSION INTERNATIONALE

POUR LA RÉFORME DE LA NOMENCLATURE CHIMIQUE

réunie à Genève du 19 au 22 avril 1892

1. A côté des procédés habituels de nomenclature, il sera établi pour chaque composé organique un nom *officiel* permettant de le retrouver sous une rubrique unique dans les tables et dictionnaires.

La Commission exprime le vœu que les auteurs prennent l'habitude de mentionner dans leurs mémoires, entre parenthèses, le nom officiel à côté du nom choisi par eux.

2. On décide de ne s'occuper, pour le moment, que de la nomenclature des composés de constitution connue, et de remettre à plus tard la question des corps de constitution inconnue.

I. Hydrocarbures

3. La désinence *-ane* est adoptée pour tous les hydrocarbures saturés.

4. Les noms actuels des quatre premiers hydrocarbures normaux saturés *(méthane, éthane, propane, butane)* sont conservés; on emploiera les noms tirés des nombres grecs pour ceux qui ont plus de quatre atomes de carbone.

5. Les hydrocarbures à chaîne arborescente sont regardés comme dérivés des hydrocarbures normaux, et on rapportera leur nom à la chaîne normale la plus longue qu'on puisse établir dans leur formule, en y ajoutant la désignation des chaînes latérales.

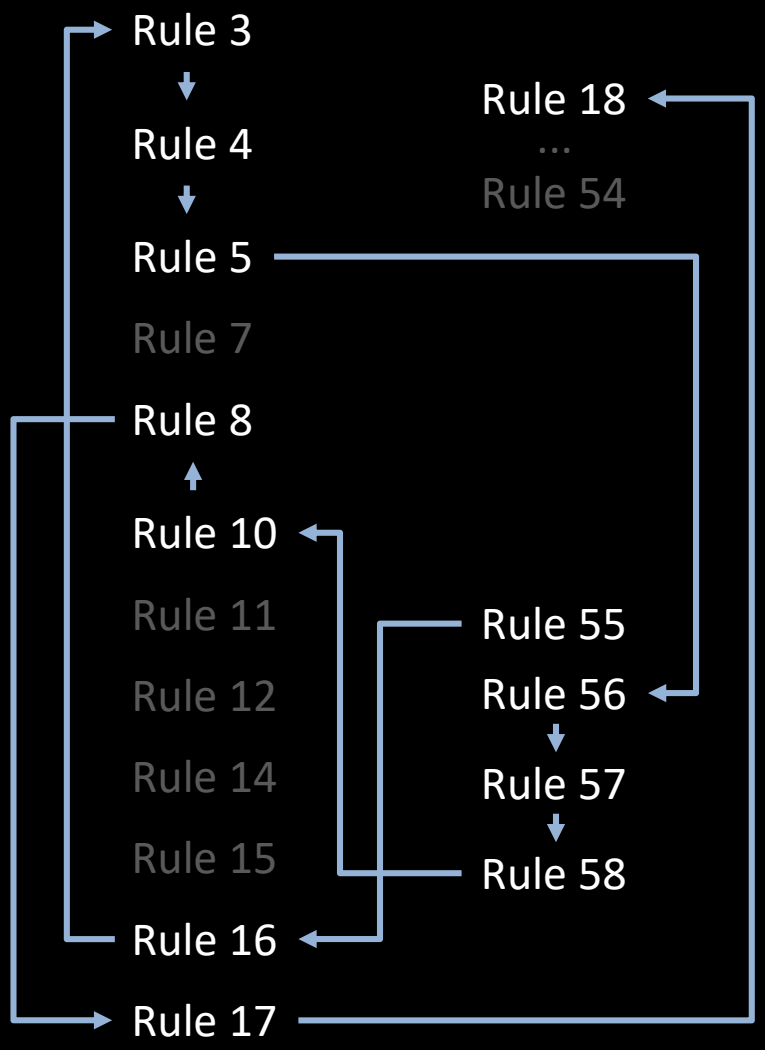
$$\begin{matrix} CH_3 \\ CH_2 \end{matrix} > CH - CH_3$$ Méthylpropane.

6. Lorsqu'un radical hydrocarboné est introduit dans une chaîne latérale, on emploiera *métho-, étho-*, etc., au lieu de *méthyl-, éthyl-*,

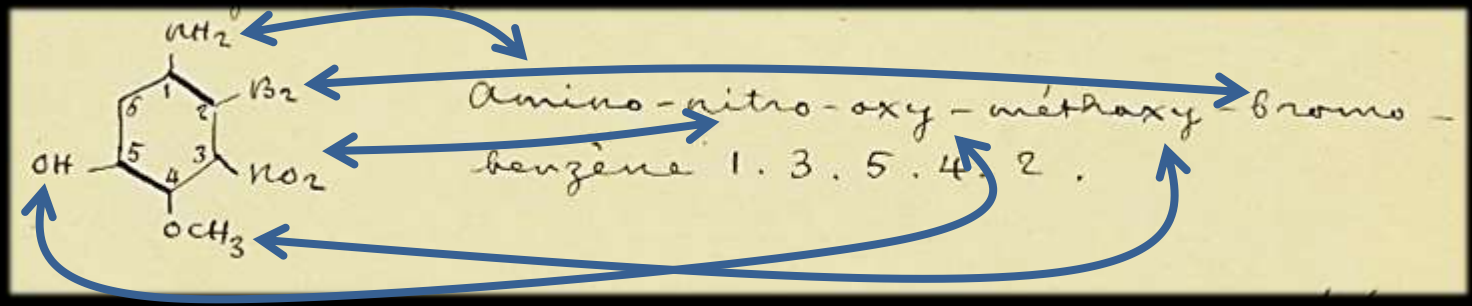
"An official name will be established for each organic compound, so that it can be looked up under a unique heading in indexes and reference works."

- “The official name of the compound is a faithful translation of its molecular structure, representing it just as the structural formula does.”

Amé Pictet, “Le Congrès International de Genève Pour La Réforme de La Nomenclature Chimique,” *Les archives des sciences physiques et naturelles* 27 (May 1892): 485–520, on 491.



Amé Pictet, Minutes of the Geneva Congress (manuscript), 176, Bibliothèque de Genève, Ms. Fr. 3423.



- “The official name of the compound is a faithful translation of its molecular structure, representing it just as the structural formula does.”

- “Concerns about brevity and harmoniousness in word choice had to be downgraded.”

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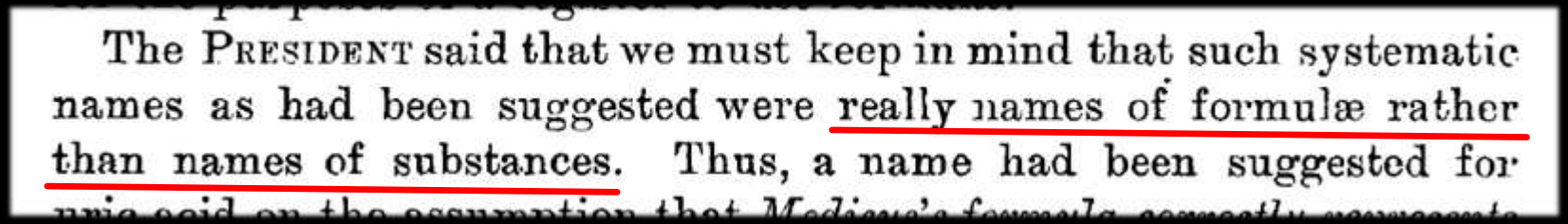
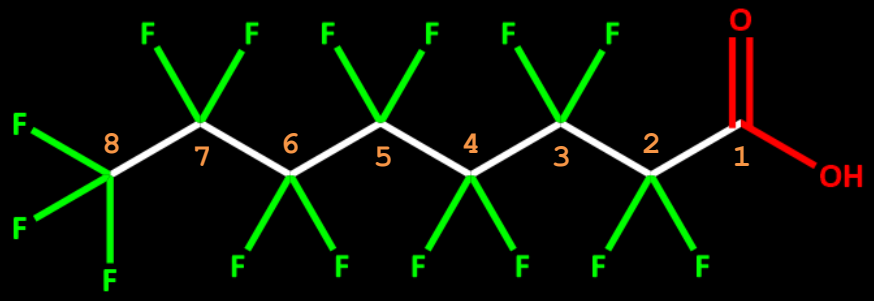
- 
The PRESIDENT said that we must keep in mind that such systematic names as had been suggested were really names of formulæ rather than names of substances. Thus, a name had been suggested for

Alexander Crum Brown, quoted in *Proceedings of the Chemical Society*, 16 June 1892.


$C_4H_8F_2$
NOMENCLATURE CHIMIQUE 1892-1992
90
HELVETIA
BURKARD WALTENSPÜL
1992
COURVOISIER
small molecule
Ceci n'est pas une ~~pipe~~.

- "The official name of the compound is a faithful translation of its molecular structure, representing it just as the structural formula does."



- "Concerns about brevity and harmoniousness in word choice had to be downgraded."

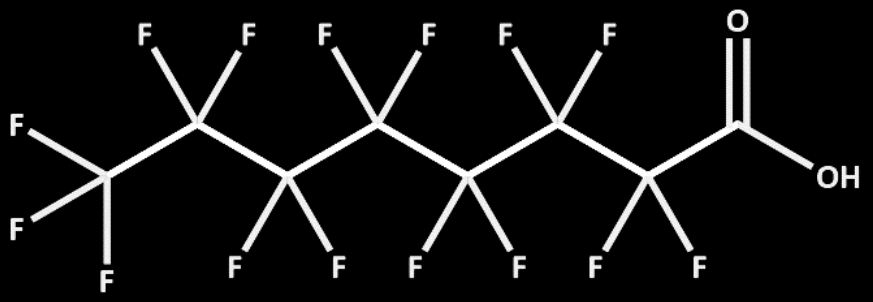
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid

- The PRESIDENT said that we must keep in mind that such systematic names as had been suggested were really names of formulæ rather than names of substances. Thus, a name had been suggested for

The Systematic Ideal

One chemical
(material substance)

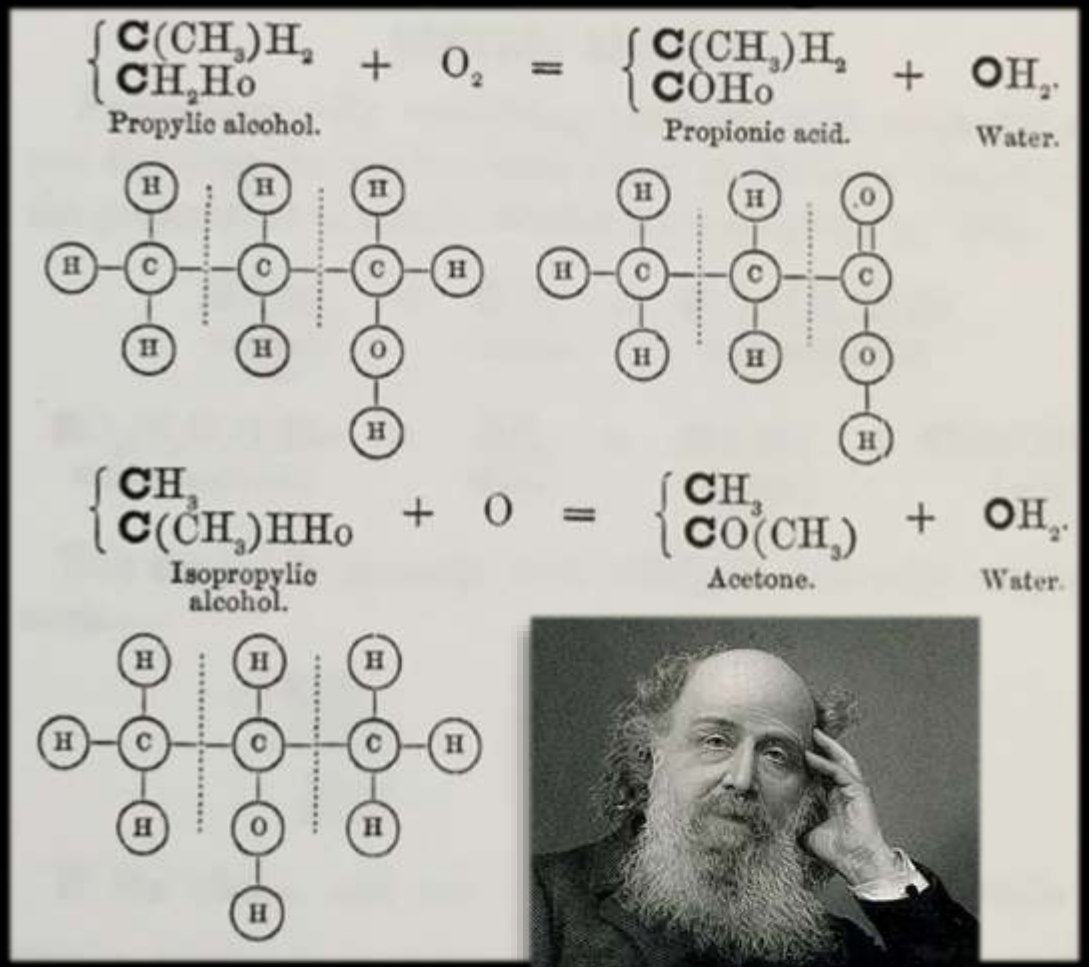
One molecular structure
(diagram)



One systematic name

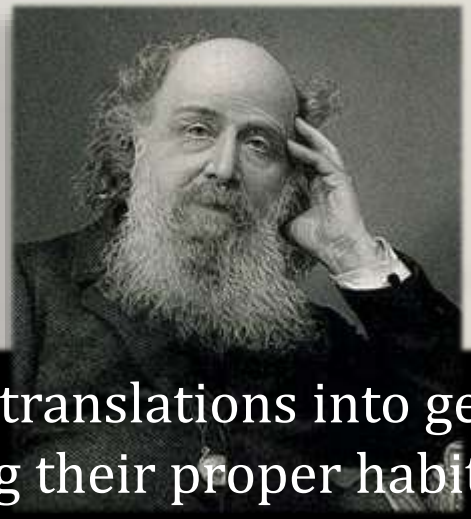
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid

A chemical history of graph theory



"The more I study Dr. Frankland's wonderfully beautiful little treatise… travelling my eye up and down the illustrated pages of "the Notes," I feel as Aladdin might have done in walking in the garden where every tree was laden with precious stones."

James Joseph Sylvester, "On an Application of the New Atomic Theory," 1878.



"**Chemical graphs**… translations into geometrical forms of priorities and sequences having their proper habitat in the sphere of order."

Chemico-Linguistics: Computer Translation of Chemical Nomenclature

If we cannot solve the problem of translating chemical nomenclature, there would seem to be little hope for translating natural languages such as English with a machine.

Eugene Garfield, founder of ISI/Web of Science, 1961

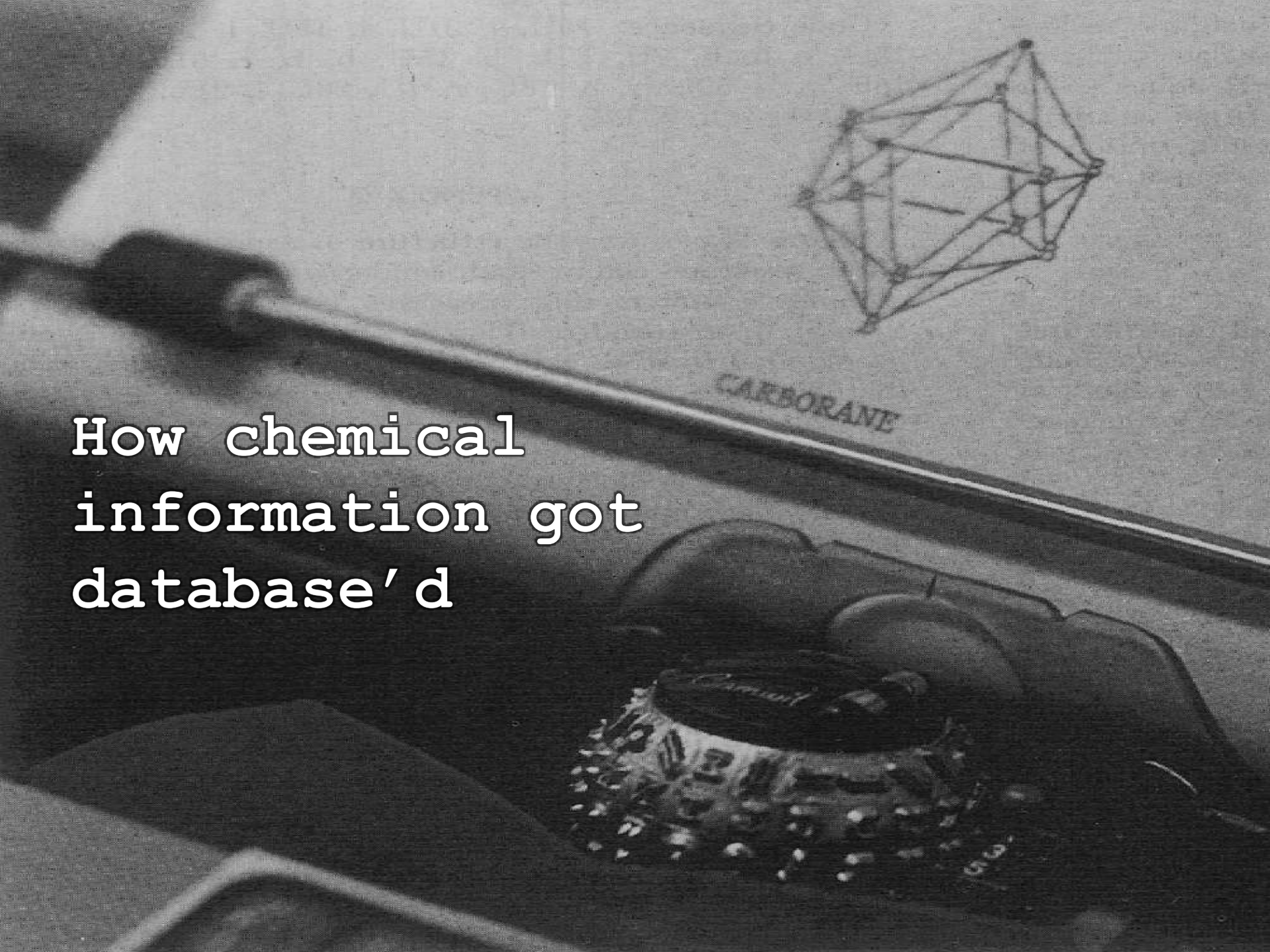
APPLICATIONS OF ARTIFICIAL INTELLIGENCE FOR ORGANIC CHEMISTRY

The DENDRAL Project

Lederberg, Djerassi, Feigenbaum et al., 1965 fwd.

9.4 THE PROSPECTS FOR AUTOMATIC SCIENCE

DENDRAL illustrates the state of the art in automatic hypothesis formation. It can lay claim to this position not merely because it has few competitors at the moment, but because it has been a thorough, sustained effort by an interdisciplinary group of

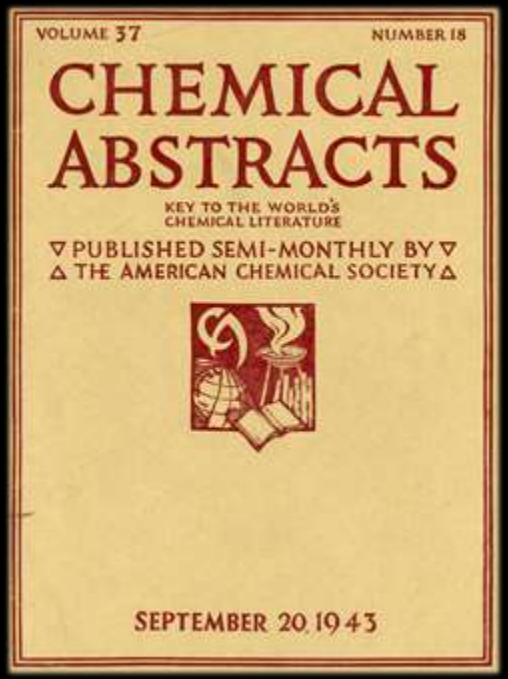


How chemical information got database'd

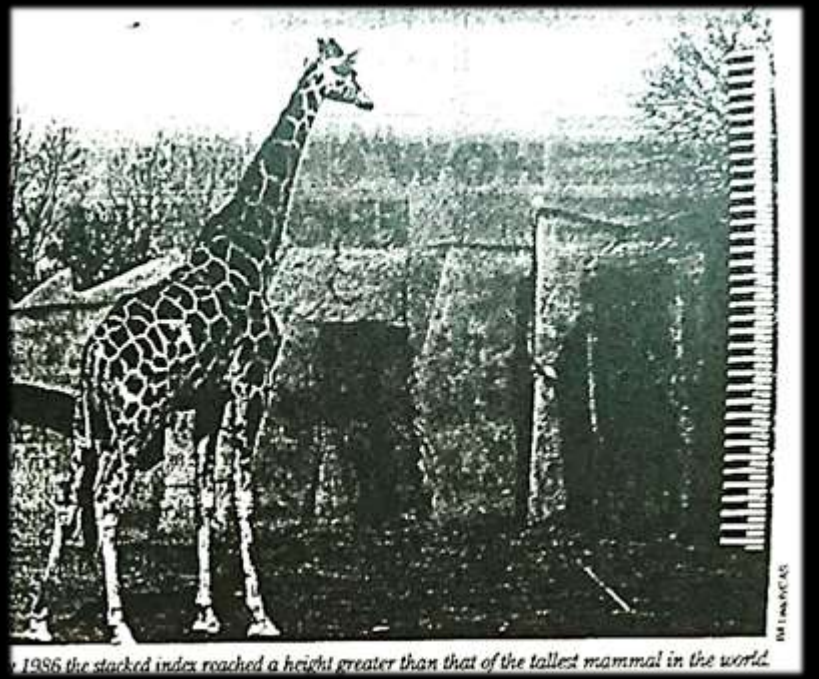
“We must organize and equip ourselves for the scientific and industrial battle that’s about to begin.

Among all of the chemist’s instruments, none is more indispensable than good books and good bibliographic literature. A chemist can no more do without these than without the balance or the thermometer.”

—Charles Moureu (1863-1929), head of French chemical warfare research during WWI and founding president of IUPAC in 1919, speaking almost exactly 100 years ago at the Interallied Chemistry Conference of April 1919



ACS employee Margot Tully surveys 19 dummy volumes, representing CA's Fifth Decennial Index, scheduled to appear over the next four-year period



1986 the stacked index reached a height greater than that of the tallest mammal in the world.

A flood of fluorocarbons: From the Manhattan Project to consumer products… and nomenclature issues

"Wanted: Jobs for a Trillion New Chemicals," *Popular Mechanics*, March 1952, 81-85.

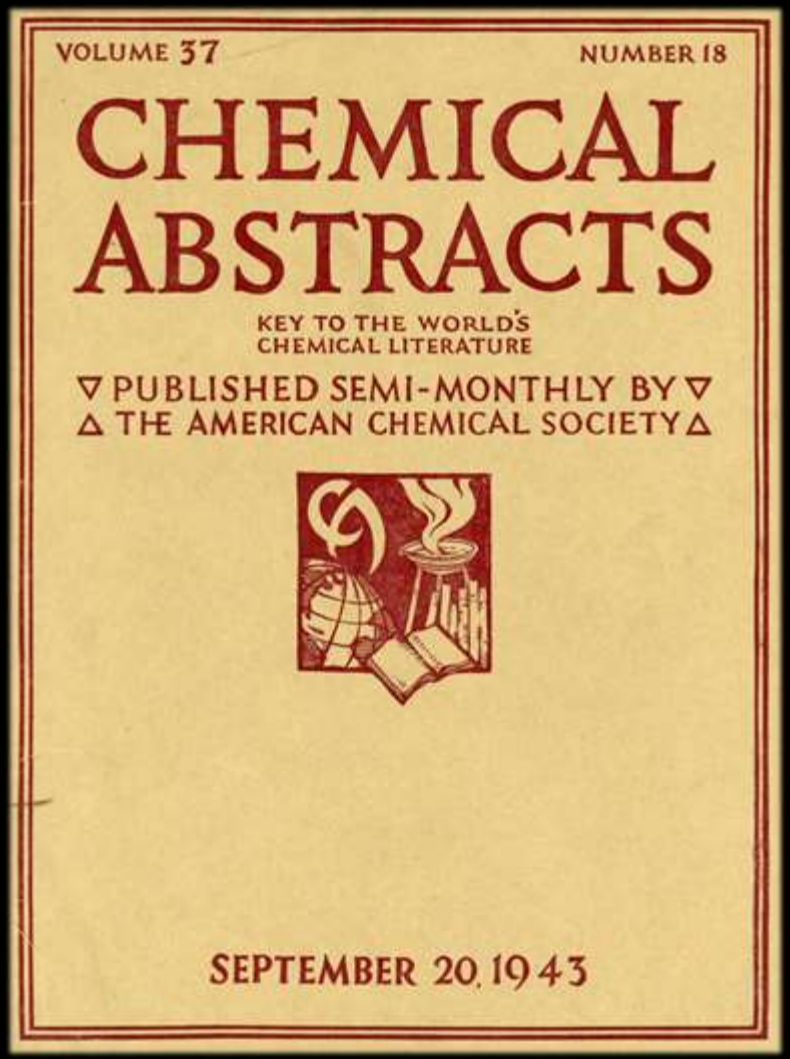
FLUORINE NOMENCLATURE . . .

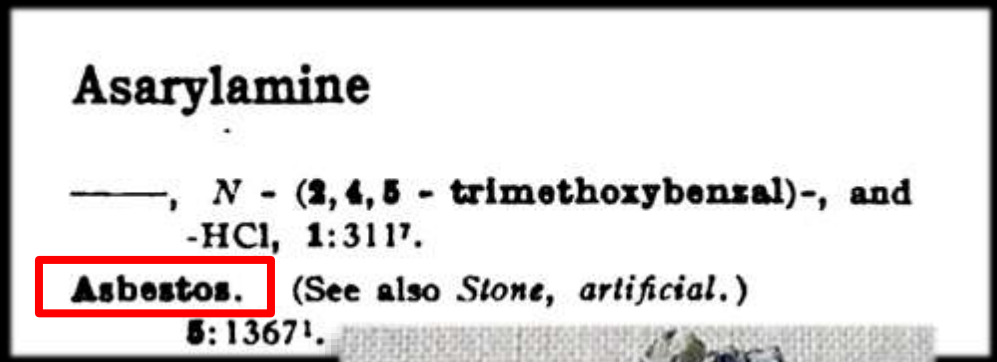
A Statement by the Editors

THE molecular construction of many of the fluoro compounds analogous to the hydrocarbon system poses a problem of nomenclature that has been a source of much inconvenience in the field. The present *Chemical Abstracts* system of nomenclature is com-

fluorine nomenclature. Also present were the editor of *Chemical Abstracts*, the chairman of the Organic Chemistry Division's committee on nomenclature, a representative of INDUSTRIAL AND ENGINEERING CHEMISTRY, and several nomenclature experts

"Fluorine Nomenclature," *Industrial & Engineering Chemistry* 39, no. 3 (March 1, 1947): 241–42.





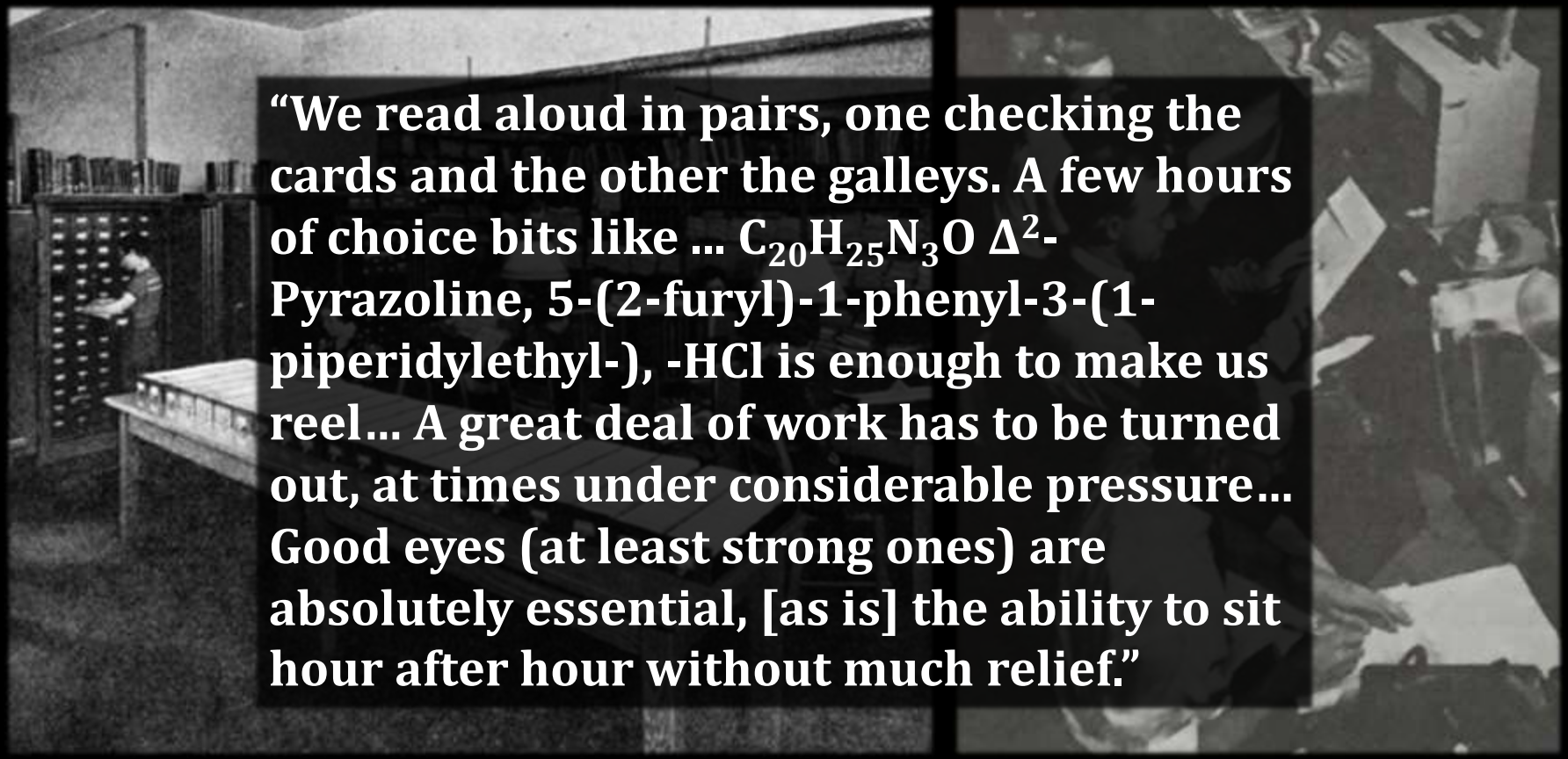
Editor-in-chief E.J. Crane: "Here, we go on the theory that rules are sometimes to be overruled by circumstances."

Crane to Leech, 26 Oct 1937, William A. Noyes Papers, 15/5/21, University of Illinois Archives, Box 14, Folder "General Correspondence, 1937–38."

The CHEMIST *at* WORK

XIV. MY WORK WITH CHEMICAL ABSTRACTS

JANET D. SCOTT



"We read aloud in pairs, one checking the cards and the other the galleys. A few hours of choice bits like ... $C_{20}H_{25}N_3O$ Δ^2-Pyrazoline, 5-(2-furyl)-1-phenyl-3-(1-piperidylethyl-), -HCl is enough to make us reel... A great deal of work has to be turned out, at times under considerable pressure... Good eyes (at least strong ones) are absolutely essential, [as is] the ability to sit hour after hour without much relief."

Index work, 1938

Index work, 1949

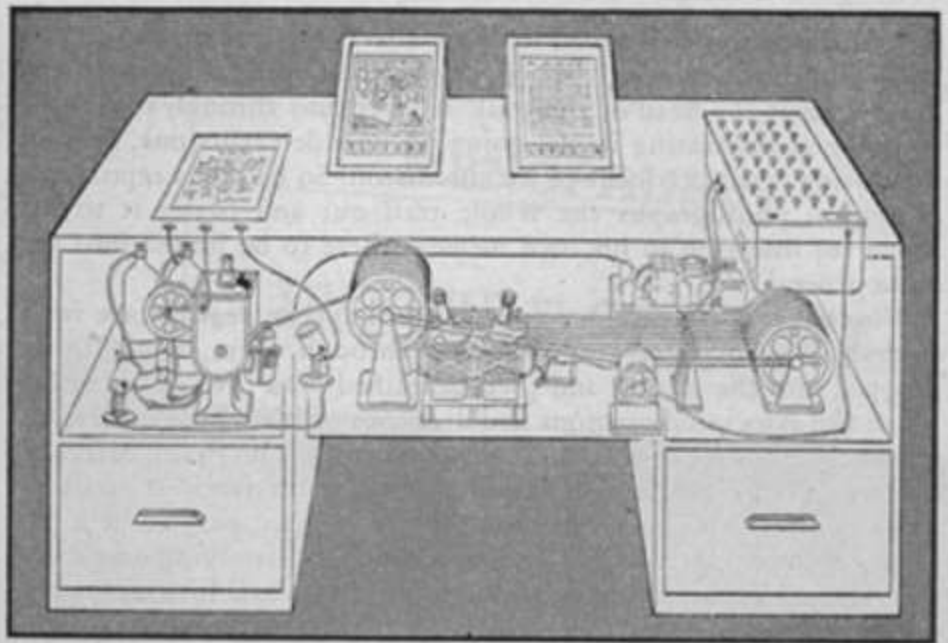
AS WE MAY THINK

A TOP U. S. SCIENTIST FORESEES A POSSIBLE FUTURE WORLD IN WHICH MAN-MADE MACHINES WILL START TO THINK

by VANNEVAR BUSH

DIRECTOR OF THE OFFICE OF SCIENTIFIC RESEARCH AND DEVELOPMENT

Condensed from the *Atlantic Monthly*, July 1945



MEMEX in the form of a desk would instantly bring files and material on any subject to the operator's fingertips. Slanting translucent viewing screens magnify supermicro-

ACS NEWS

Mostly a Research Report

The CHEMICAL ABSTRACTS Service—Good Buy or Good-by

E. J. CRANE, *Director, Chemical Abstracts Service*

Calvin Mooers
(1919-1994)

"While those interested in the indexing business are many (e.g. the patent office, the census bureau, UNESCO, large libraries), the biggest push at the moment is the American Chemical Society... the Society will need a liason [sic] between the electronics and their semantic problem."

Calvin Mooers to Howard Mooers, 27 Jan 1947, Calvin and Charlotte Mooers Papers, Charles Babbage Institute Archives, University of Minnesota, CBI 81, Box 7, Folder 7.

The Prospects for the Utilization of Informational-Logical Machines in Chemistry (USSR)*

L. I. Gutenmakher and G. E. Vleduts

French National Policy for Chemical Information and the DARC System as a Potential Tool of This Policy*

J. E. DUBOIS
The Paris VII University, 1, rue Guy de la Brosse, Paris, France

A CLUSTER OF ALGORITHMS RELATING THE NOMENCLATURE OF ORGANIC COMPOUNDS TO THEIR STRUCTURE MATRICES AND CIPHERS

G. M. Dyson

Scientific Management Ltd., Loughborough, Leicestershire, England

HOW STANDARDS PROLIFERATE:

(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC)

SITUATION:
THERE ARE
14 COMPETING
STANDARDS.

14?! RIDICULOUS!
WE NEED TO DEVELOP
ONE UNIVERSAL STANDARD
THAT COVERS EVERYONE'S
USE CASES.

SOON:

SITUATION:
THERE ARE
15 COMPETING
STANDARDS.

Chemical Abstracts Service Chemical Substances Registry

"CAS Registry"

Think: "Fingerprint"

Connection Table

Atoms		Bonds		
#	Type	From	To	Order
1	C	1	2	1
2	C	2	3	1
3	C	3	4	1
4	C	4	5	1
5	C	5	6	1
6	C	6	7	1
7	C	7	8	1
8	C	1	9	2
9	O	1	10	1
10	O	2	11	1
11	F	2	12	1
12	F	3	13	1
13	F	3	14	1
14	F	4	15	1
15	F	4	16	1
16	F	5	17	1
17	F	5	18	1
18	F	6	19	1
19	F	6	20	1
20	F	7	21	1
21	F	7	22	1
22	F	8	23	1
23	F	8	24	1
24	F	8	25	1
25	F			

Think: "social security number"

Registry Number

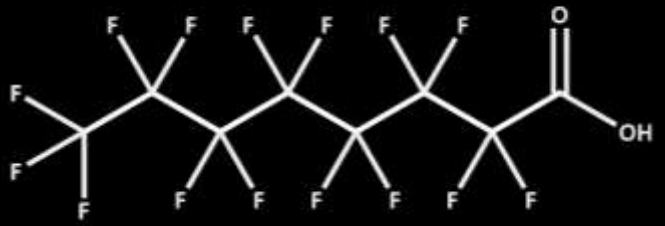
335-67-1

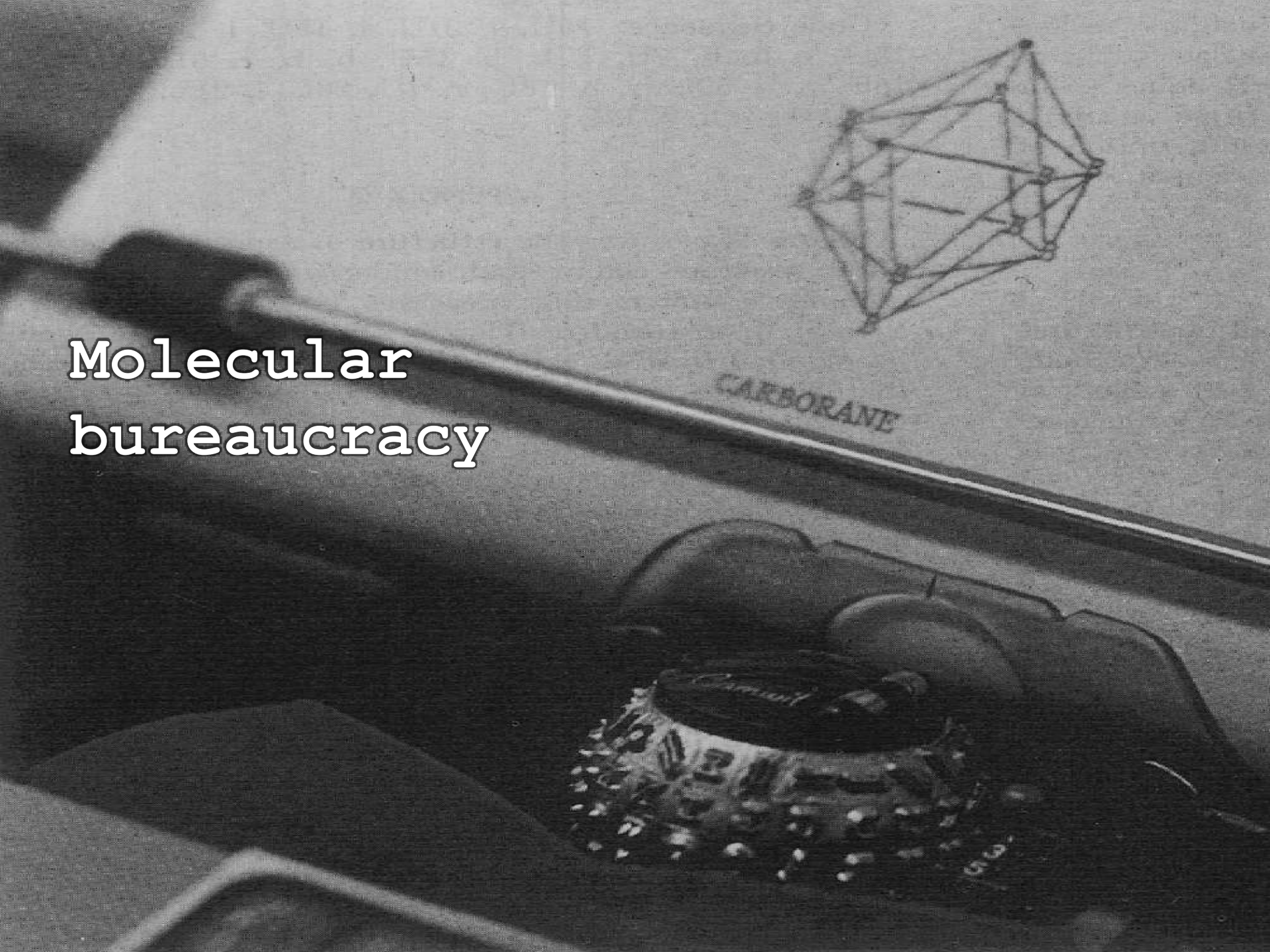
Data

Articles

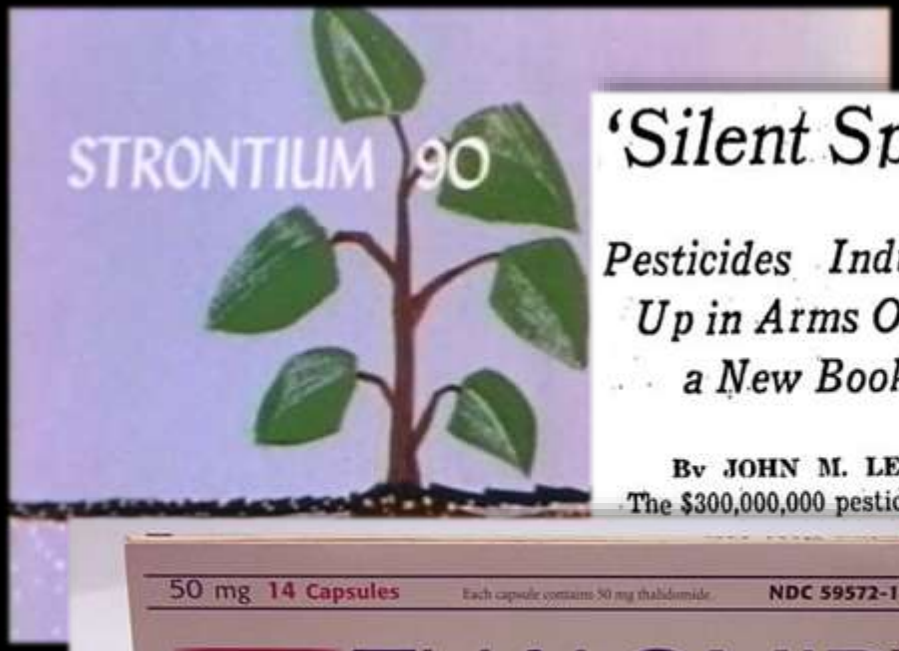
Patents

Data entry





Molecular bureaucracy



'Silent Spring' Is Now Noisy Summer

Pesticides Industry Up in Arms Over a New Book

By JOHN M. LEE

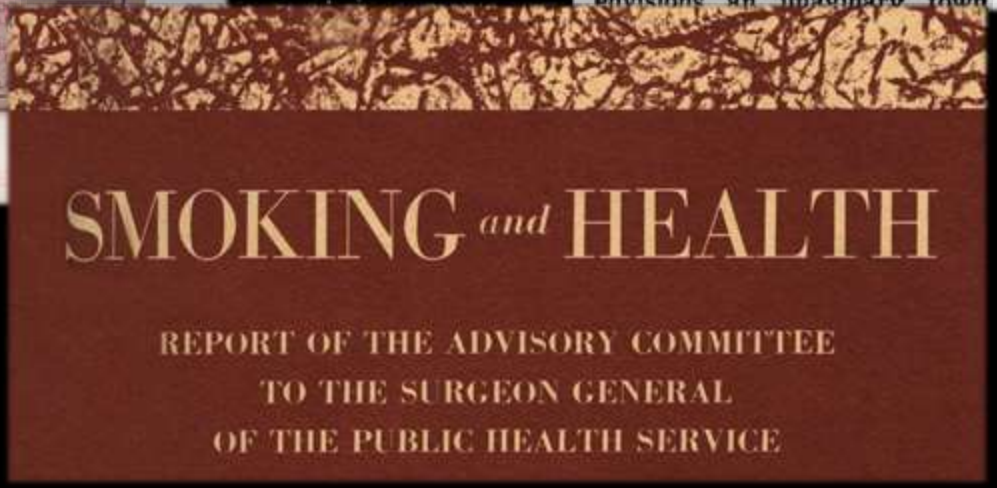
The $300,000,000 pesticides in-

Rachel Carson Stirs Conflict—Producers Are Crying 'Foul'

fending the use of their products. Meetings have been held in Washington and New York. Statements are being drafted and counter-attacks plotted.

A drowsy midsummer has suddenly been enlivened by the greatest uproar in the pesticides industry since the cranberry scare of 1959.

Miss Carson's new book is entitled "Silent Spring." The title is derived from an idealized situation in which Miss Carson envisions an imaginary town



Lose-dose, high-profile: chronic toxicity concerns, late 1950s-early 1960s.

CHEMICAL & ENGINEERING
NEWS

JUNE 7, 1965

CAS to Study Registry of Chemical Compounds

R&D project under NSF contract could lead to computer-based information system

The American Chemical Society and the Federal Government last week came to terms on an R&D project that could well make or break the concept of national systems for handling scientific and technical information. Under a two-year, $2 million contract with the National Science Foundation, the ACS's Chemical Abstracts Service, under director Dale Baker, will attempt to prove the technical feasibility of a computer-based "registry of chemical compounds." This registry system is to be the foundation

been published on them before and, if so, what. Each unique compound fed into the system will be given its own identification number. That number will be the key for locating other information about the compound stored elsewhere in the computer system.

Information stored on computer tapes in addition to the registry number will include a detailed description of the compound's structure, its molecular formula, any names (systematic, trivial, or trade) and laboratory codes

Donald F. Hornig
A critical experiment

Solution: "a much more coordinated and more complete computer-based file of toxicological information"… a "total body of chemical and biological information.

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NATIONAL CANCER INSTITUTE

ATOMIC ENERGY COMMISSION UNITED STATES OF AMERICA

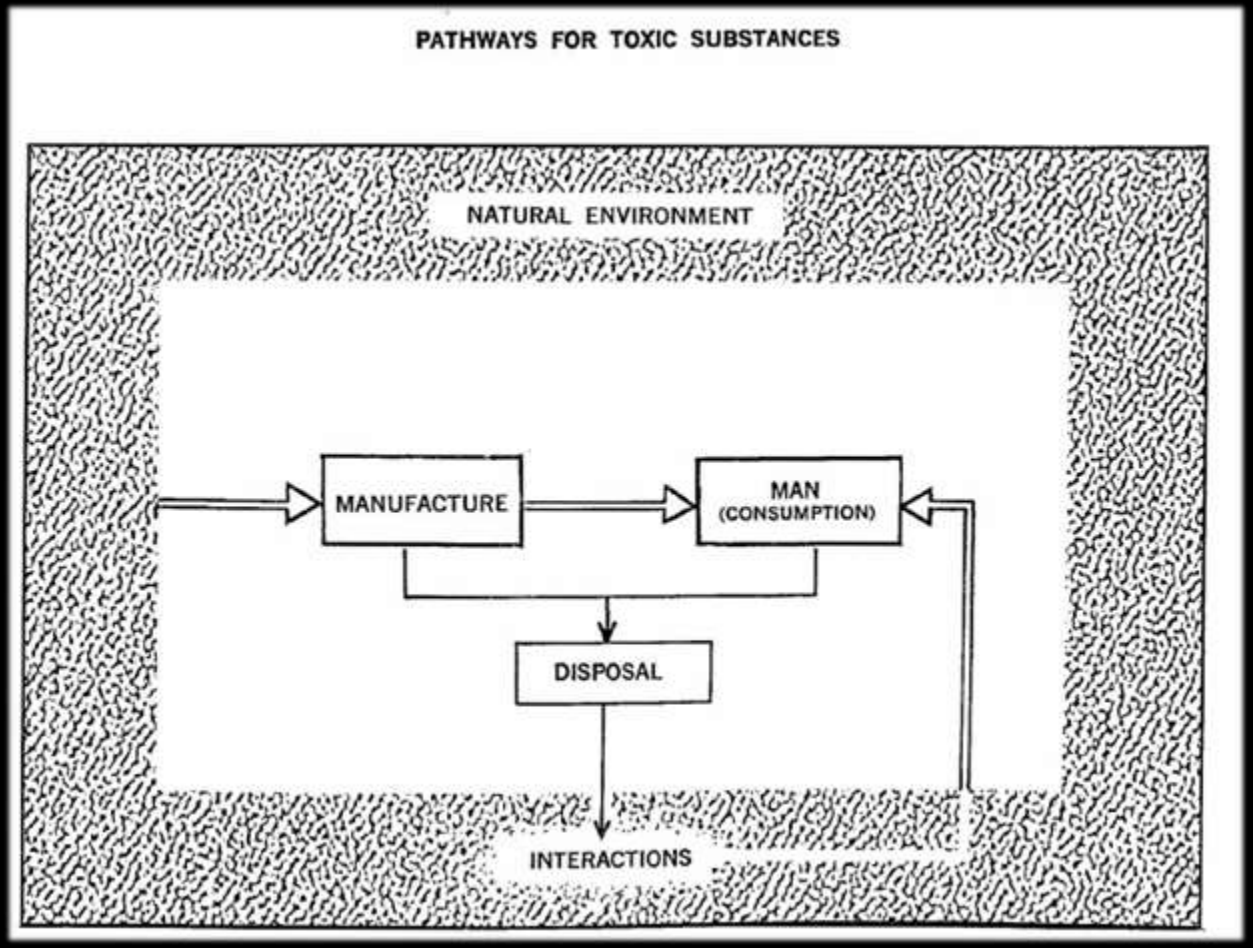
…

NIH computing expert, 1976:

"An emerging pattern of international cooperation seems to have ensured the fact that all molecular structure files will be linked to the CAS Registry Number in the future….

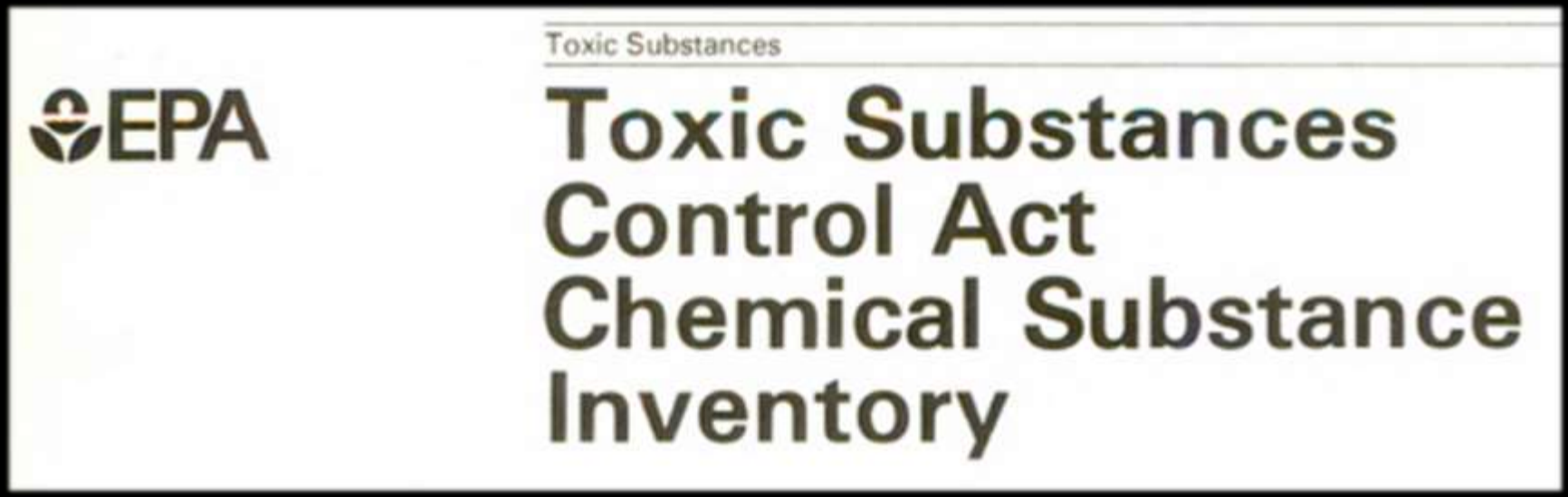
Regardless of how this identifier came into existence, it is clear that the future evolution of chemical (structure-related) information is bound to the CAS universal identifier. Scientists should think of data as being linked to the body of chemical information by the universal identifier."

Chemical Holism



Toxic Substances (1971 Nixon administration report)

"Standard-setting, monitoring, and control can often be done more efficiently and rationally if attention is focused on the particular substance."



"This list is the foundation on which all toxic substances control will be based."

Frederick H. Siff, "Inventory Information in the Chemical Abstract Service," in *2nd Annual ADP Conference* (Washington: EPA, 1977), H-11.

"The inventory describes what is in the universe.... The processing of the inventory will take place at the Chemical Abstract Service [sic]."

EPA

Toxic Substances

Toxic Substances Control Act Chemical Substance Inventory

"This list is the foundation on which all toxic substances control will be based."

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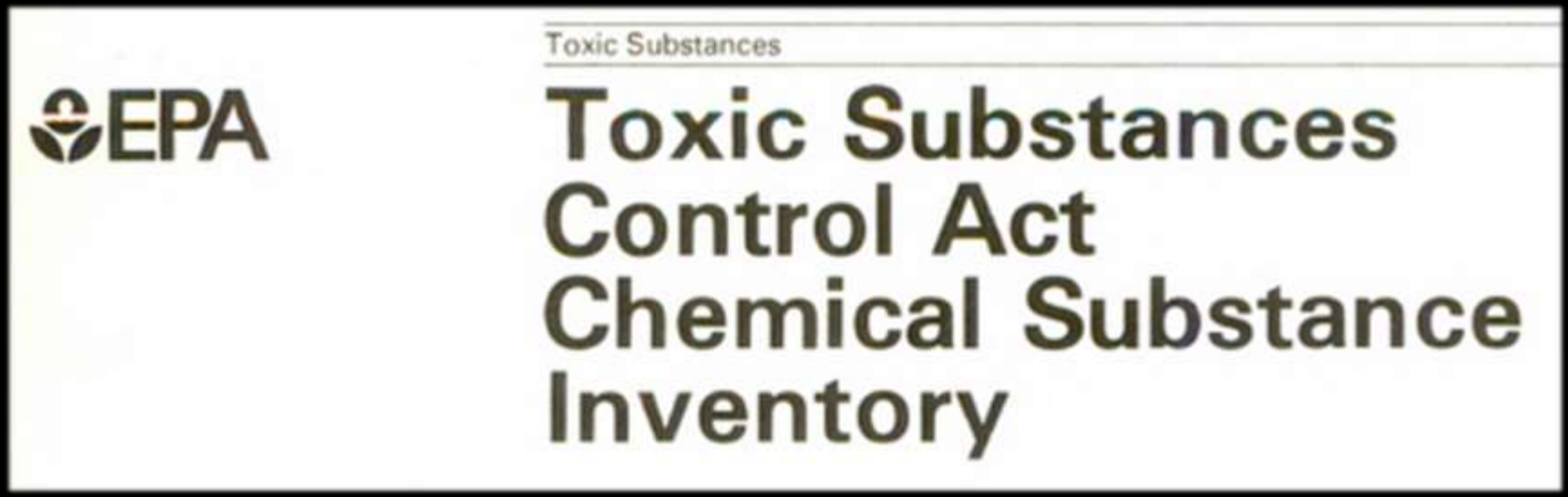


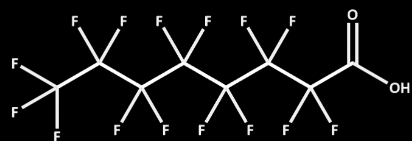
"This list is the foundation on which all toxic substances control will be based."

UVCBs!

"The CAS means of identification led to all kinds of technical issues and nomenclature issues that took huge amounts of time and resources…. It just has nothing to do with protecting health and safety. It just got to be a bureaucratic exercise."

Steven Jellinek, head of EPA Office of Toxic Substances, 1977-1981 (in 2010)

Molecular Bureaucracy



2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid

Connection Table

Atoms #	Type	Bonds From	To	Order
1	C	1	2	1
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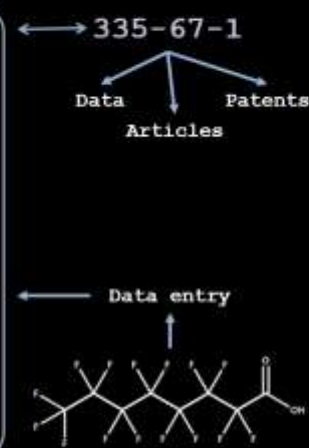
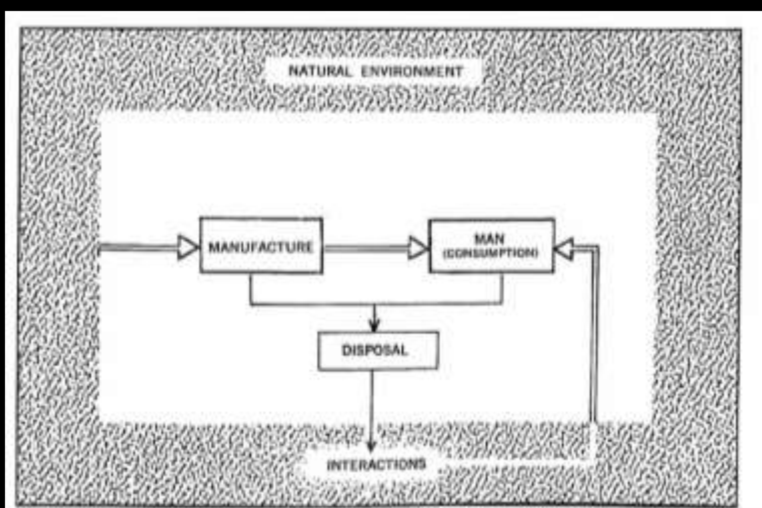
10	O	2	11	1
11	F	2	12	1
12	F	3	13	1
13	F	3	14	1
14	F	4	15	1
15	F	4	16	1
16	F	5	17	1
17	F	5	18	1
18	F	6	19	1
19	F	6	20	1
20	F	7	21	1
21	F	7	22	1
22	F	8	23	1
23	F	8	24	1
24	F	8	25	1
25	F			

Registry Number





NEWS

CAS to Study Registry of Chemical Compounds

R&D project under NSF contract could lead to computer-based information system

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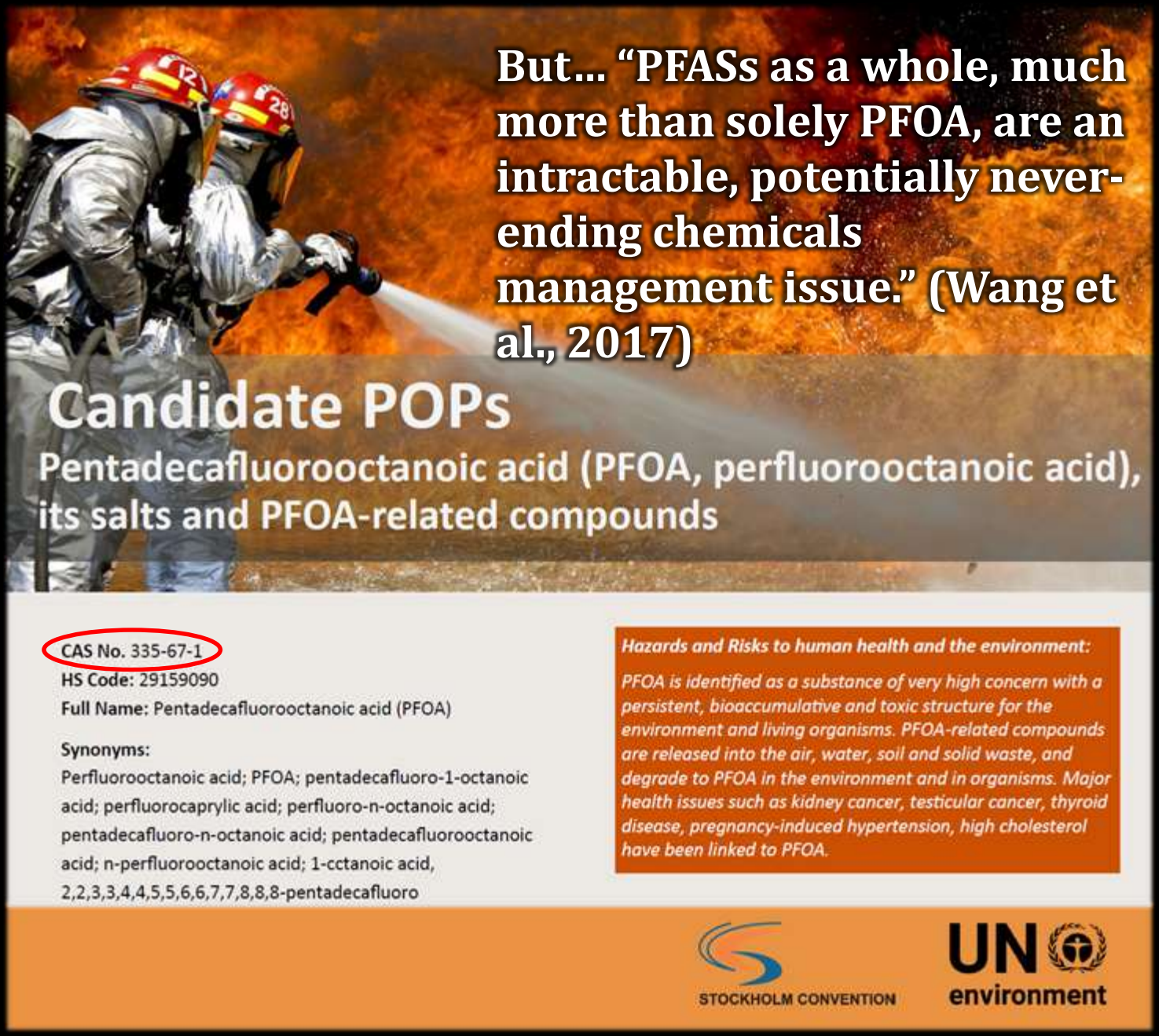
But… "PFASs as a whole, much more than solely PFOA, are an intractable, potentially never-ending chemicals management issue." (Wang et al., 2017)
Candidate POPs
Pentadecafluorooctanoic acid (PFOA, perfluorooctanoic acid), its salts and PFOA-related compounds
CAS No. 335-67-1
HS Code: 29159090
Full Name: Pentadecafluorooctanoic acid (PFOA)
Synonyms:
Perfluorooctanoic acid; PFOA; pentadecafluoro-1-octanoic acid; perfluorocaprylic acid; perfluoro-n-octanoic acid; pentadecafluoro-n-octanoic acid; pentadecafluorooctanoic acid; n-perfluorooctanoic acid; 1-cctanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro
Hazards and Risks to human health and the environment:
PFOA is identified as a substance of very high concern with a persistent, bioaccumulative and toxic structure for the environment and living organisms. PFOA-related compounds are released into the air, water, soil and solid waste, and degrade to PFOA in the environment and in organisms. Major health issues such as kidney cancer, testicular cancer, thyroid disease, pregnancy-induced hypertension, high cholesterol have been linked to PFOA.
STOCKHOLM CONVENTION
UN environment

“The simplification of ontology has led to the enormous complication of epistemology.”

...So three cheers for complicated ontologies!

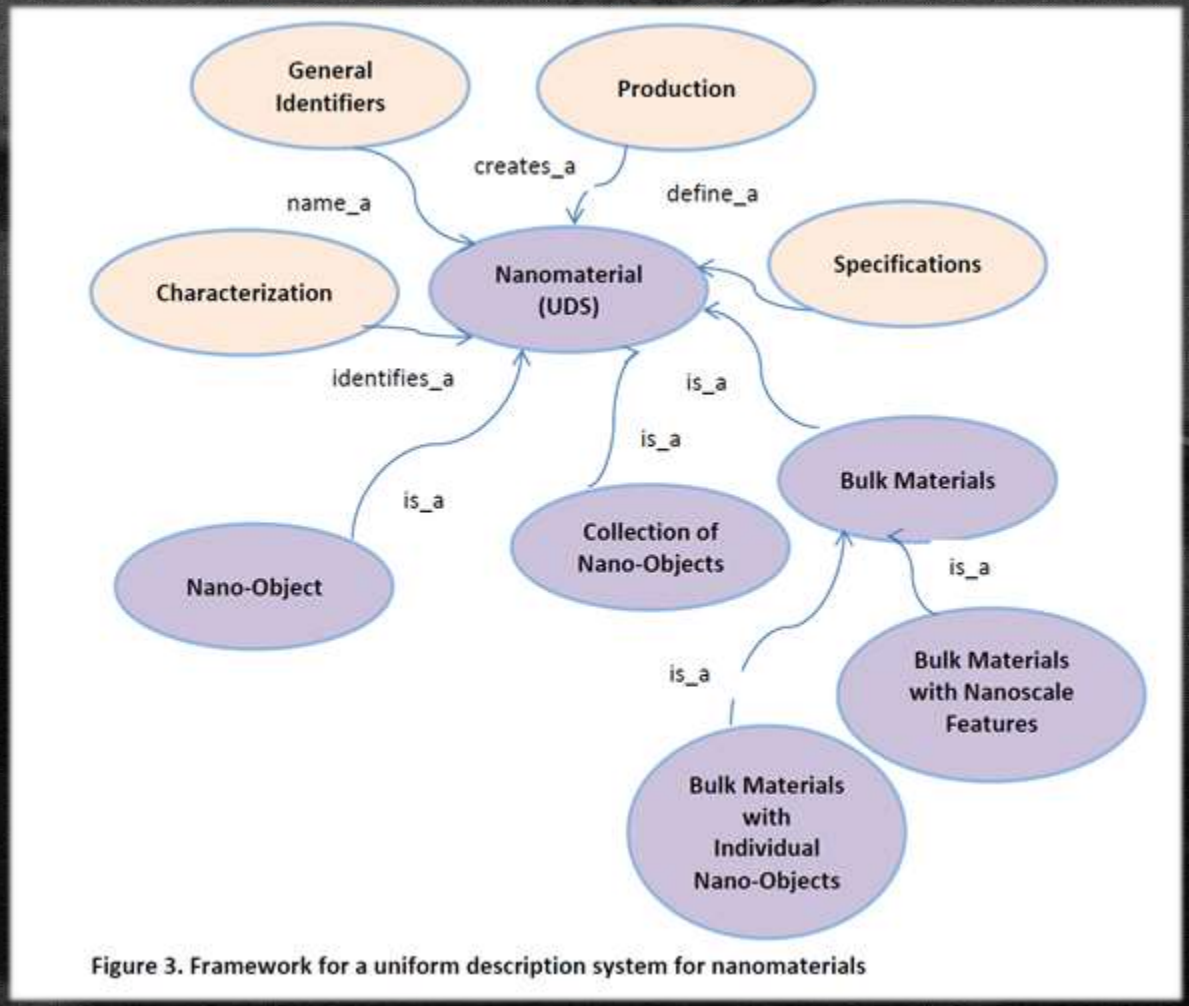

Figure 3. Framework for a uniform description system for nanomaterials

Thank you!

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evanheplersmith.com

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