Molecular Bureaucracy A Chemical History of Data

Data Then and Now University of Washington February 12, 2020

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Being Digital & Being Material





The Environmental History of Computing

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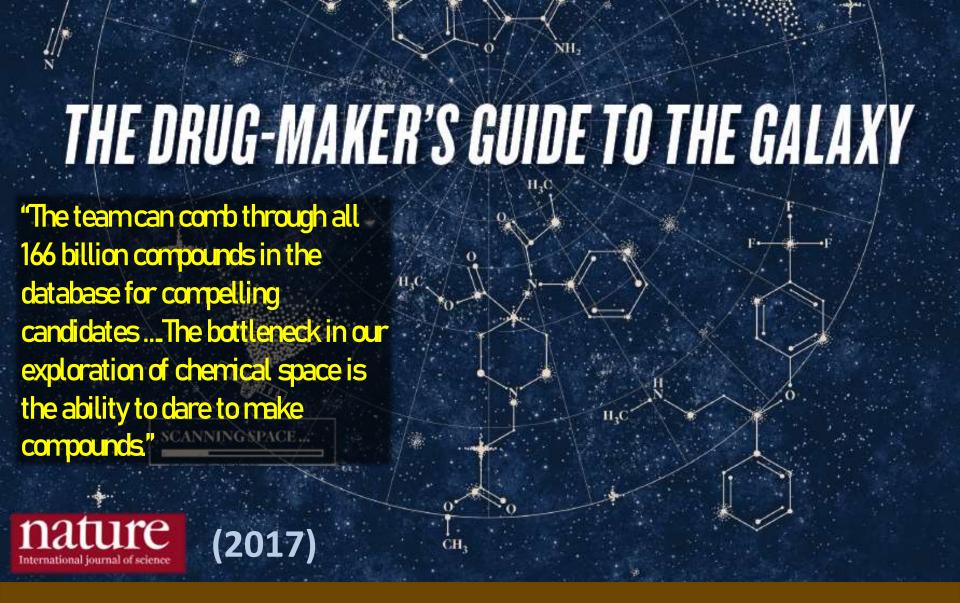
NATHAN ENSMENGER

Being Digital & Being Material



My interest: how <u>digital</u> information systems and data structures enact (attune to, interact with, shape (Mol 2002)) <u>material</u> chemical substances in identifying, representing, and classifying them, especially via bureaucratic & informatic re-use/re-purposing





THE DRUG-MAKER'S GUIDE TO THE GALAXY

ChemMaps.com

DrugMap

DSSToxMap

Tox21Map

Generate the 3D Map

Select up to 5 features you would like put on the map:

Chemical classification

- EPA category
- LD50 (mg/kg)

Toxicology prediction

- Acute Tox (very toxic)
- Acute Tox (no toxic)
- Acute Tox (EPA)
- Acute Tox (GHS)
- Acute Tox (LD50)
- Estrogen Receptor activity (Agonist)
- Estrogen Receptor activity (binding)
- Hepatic clearance

■ Androgen Receptor Activity (Antogonist) Melting Point (C)

Physicochemical prediction

- Androgen Receptor Activity (binding)
- Plasma fraction unbound
- Henry's Law constant (atm-mol3/mole)
- KM (biotransformation rate)
- Log Octanol/air partition coefficient
- Log Soil adsorption coefficient (L/Kg)
- Log Fish bioconcentration factor
- LogD
- LogP

- Pka acid
- Pka basic
- Biodegradability
- HPLC retention time
- Log vapor pressure (mmHg)
- Log Water solubility
- Log Atmospheric constant (cm3/molsec)
- Biodegradation half-life
- Boiling Point

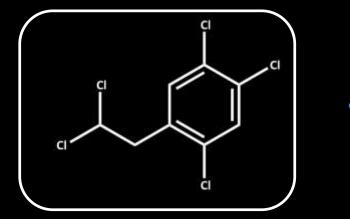
Descriptors

- MW E
- Lipinski Failures

Generate Tox21Map

Example: Quantitative Structure-Activity Relationships (QSAR)

Chemical structure



Numerical parameters

$$\sigma_1 = 0.28$$
, $\sigma_2 = 0.84$, ...

 π_1 , π_2 , π_3 , ...

 ρ_1 , ρ_2 , ρ_3 , ...

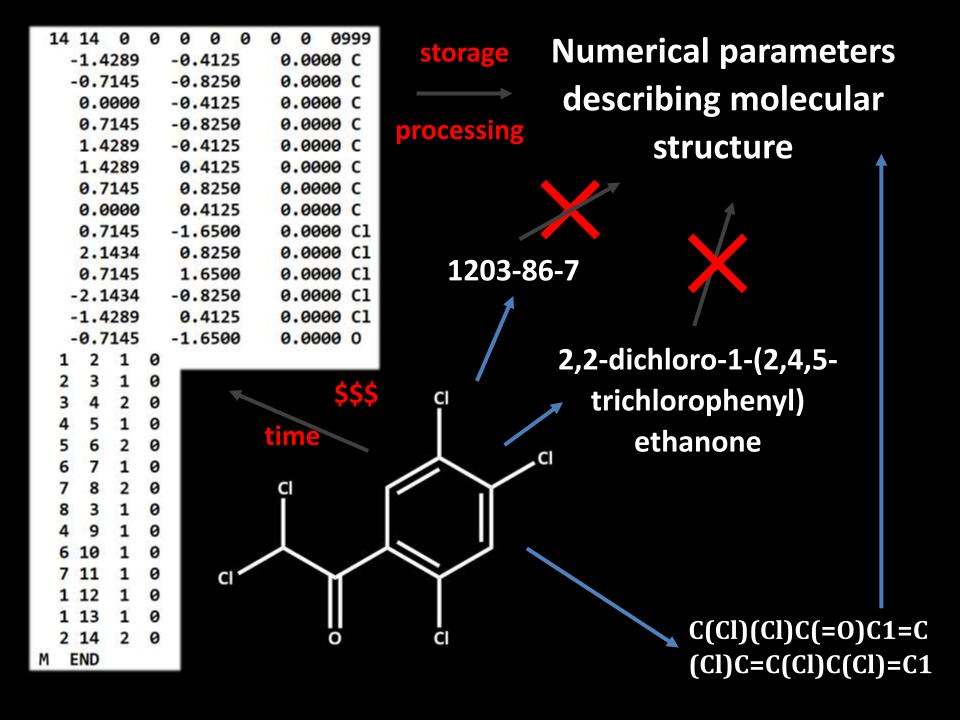
Predicted
biological effects of
new chemicals in
this structural
family



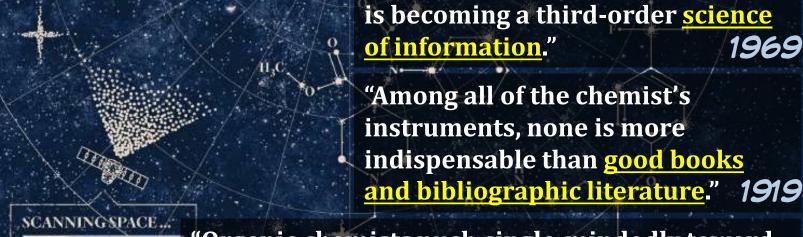
For a family of chemicals:

Parameters + reference data +

regression = QSAR



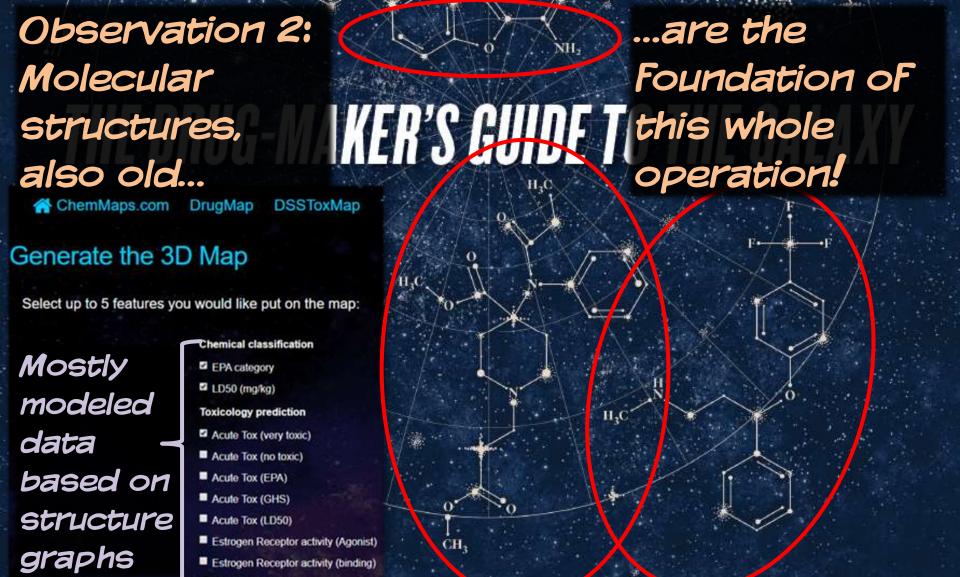
Observation 1: This argument is old THE DRUG-MAKER'S GUIDE TO THE GALAXY



"Organic chemists push single-mindedly toward the goal of striking gold.... Given the seemingly inexhaustible wealth of the land, the work inevitably becomes somewhat mechanical." 1887

"The material science of chemistry

1969



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

Hepatic clearance

The Molecular Ideal (b. 1892)

One chemical (material substance)



One structural formula (representation)

One systematic name (identity)

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

Chemicals governance







Chemical information infrastructure (digital)

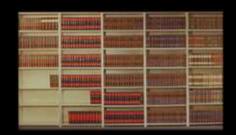






Chemical information infrastructure (print)



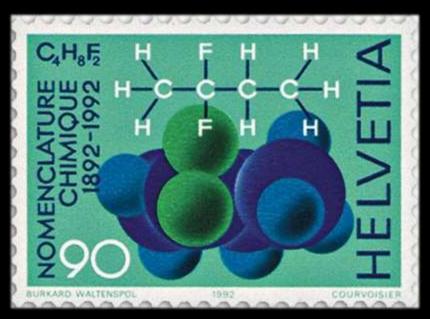


UNION INTERNATIONALE
DE LA CHIMIE PURE ET APPLIQUÉE

(Book in progress...)

Compound Words

Chemists, Information, and the Synthetic World







| 第五集 | J | 科學名詞 | 審查會所審定之有機化學 | 名詞草案 4 | 479 |
|------|--------------------------------|-------------------|-----------------------|-------------|-----|
| | C ₅ H ₁₂ | Pentane | | 五炭烷 | |
| | GH _t , | Hexane | | 六炭烷 | |
| 2. 7 | 有支練 | 之幹線,命名 | 名時先舊支線,次及幹練支(| 幹之分別,在練之長短。 | 長 |
| 者 | 36 幹,短 | 者為支.支制 | 乘之名後本應加基字. 个但: | 省去炭宁,不另加基字 | IJ |
| 示 | 與幹練 | 區別例如:- | - | | |
| - | CHa⊷ÇI | H-CH ₂ | | | |
| | ÇF | ł, | Methylpropane | 一烷三炭 | 烷 |

Some arguments

- The molecular ideal originated as a way to organize printed chemical bibliographies, mostly in order to support chemical industry R&D
- It (purposefully!) did not address all sorts of materials & ways of thinking about materials important to chemists
- It had historically-grounded affinities with mechanical methods for information retrieval and processing
- Mechanizing compilation of chemical reference books

 → chemical databases that presumed/suggested the
 universality of the molecular ideal → computational
 methods, information infrastructures, and
 administrative procedures that took the molecular ideal
 for granted and/or built on it ("molecular bureaucracy")

Some helpful notes from media philosophy and anthropology

"Ontology, whatever else it is, is usually just forgotten infrastructure." (Peters, *The Marvelous Clouds*, 2015)

"Without ideality, a plan, a map, a model, an ideal, a direction, or a theme, materiality could not materialize itself."

(Grosz, *The Incorporeal*, 2017)

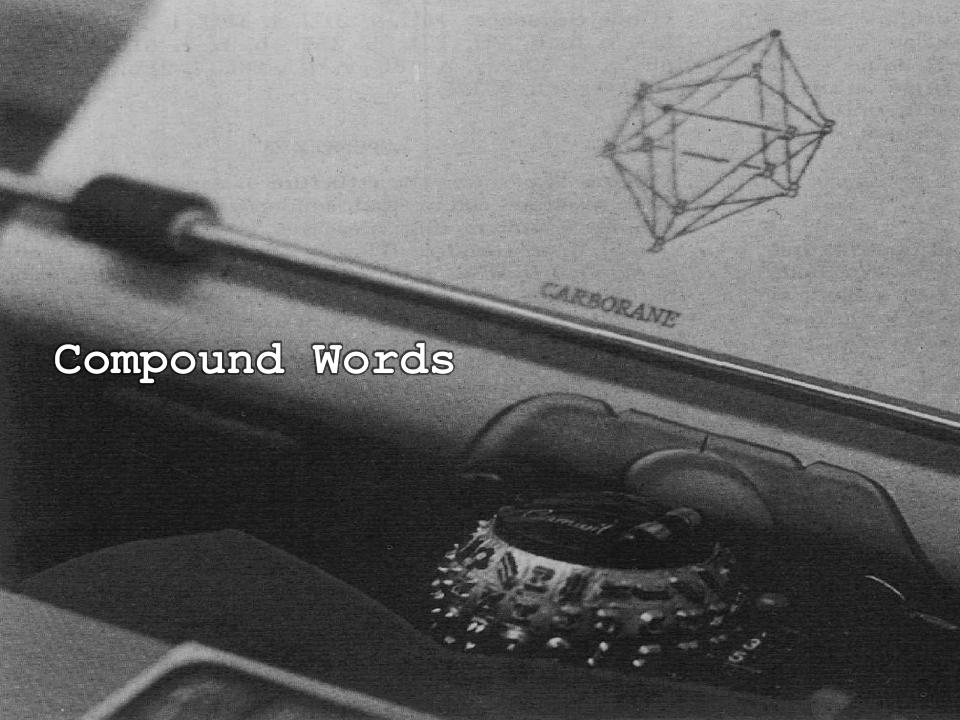
"The simplification of ontology has led to the enormous complication of epistemology." (Viveiros de Castro, "Exchanging Perspectives", 2004)

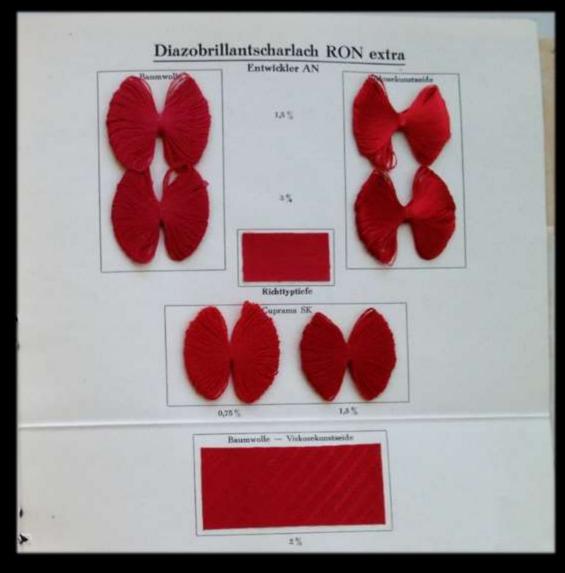
Our next half hour, aka the sampler platter...

1. "Compound words," c. 1865-1965

- 2. The chemical history of graph theory
- 3. Data structures, interfaces, & artificial experts
- 4. Molecular bureaucracy/chemical environment

5. Wrap-up





Bayer coal-tar dye samples

| Agurin | | | | | | Figs |
|--|--------|-------------------|----|----|-----|------|
| Aristochin | | | | | 7// | 5 |
| Aristol | | | | | | 8 |
| Aspirin | | | | | | 11 |
| and the same of th | - | | | | | 18 |
| Acnir | ir | , | | | | 20 |
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| Hedonal | | | | | | 33 |
| Helmitol . | · Inni | 1 | | | | 39 |
| Heroin hydroel | - | | | | | 42 |
| Hero | in | | | | | 49 |
| Hero | 111 | | | 20 | 100 | 52 |
| Mesotan | | mari ² | | | | 56 |
| Milk Somatose | | | | | 7 | 58 |
| Phenacetine-Ba | ver | | | | - | 64 |
| Piperazine-Bay | er | | | | *** | 67 |
| Protargol . | | | | | | 69 |
| Salicylate of S | alog | uini | ne | | | 76 |
| Saloquinine | | | | | | 77 |
| Salol | | | | | | 79 |
| Salophen | 41 14 | | | | | 81 |
| Somatose | 90 AT | | | | 20 | 84 |
| Sulfonal-Bayer | | | | | | 90 |
| Tannigen | 10 15 | | | 7 | | 92 |
| Tannopin | 10. 60 | 2 | | | W | 96 |
| Theoein | 0 60 | | - | | | 98 |
| Theoein-Sodiur | n . | | - | | | 104 |
| Trional-Bayer | (F) F | | | | | 101 |
| Indications . | | | | | | 105 |

Catalog of Bayer drugs available in the US, circa 1905

$$C_3H_8O$$
 $C_3H_6O_2$ propyl + — Propionic alcohol oxygen acid

What gives? (1830s-60s European organic chemistry)

Isomers:
same
composition,
different
properties

Way diFFerent reaction products

Isopropyl + ---- acetone alcohol oxygen

 C_3H_8O C_3H_6O

definite manner by adding "n" to the true type CM4. C...O...OH

In like manner the butyle alcohol is to be viewed as

"Constitutional" or "structural" formulas

Ċ...H2 C...H2

C...H3 The con-

and so on throughout all the series of these alcohols.

C... H. H. ... C

stitution of the æthers will be evident :

Ċ...H2 H3C Ċ...H2

Ċ...H³

XII. On a New Chemical Theory. By Archibald S. Couper, Esq.*

the mixed butylic-ethylic æther.

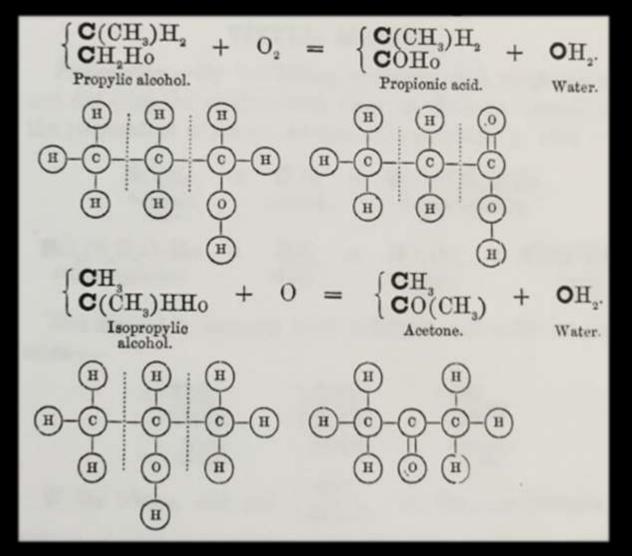
HO...O.

Formic acid is represented by the form C...O2 ; acetic acid

in like manner, C...O...OH Propionic acid is C...H2 Ċ...H^a

constitution of glycol may be represented as follows:-

(Couper, Phil. Mag., 1858) C₃H₈O



"Constitutional" or "structural" formulas

Frankland, *Lecture Notes for Chemical Students* (1866)

| Monochlorerotoms. Silber Monojodtoluol Moto 5 Mono 66 G9: Wärmeleitum 5 Mono 66 G9: Wärmeleitum 5 Mono 66 G9: Wärmeleitum 5 Mono 67 T20: Brechung 1 Chromoxychlorid, ge, 72: Bildungswäm 5 Mono 70 T22: Verh. 360; T23: Verh. 370; T24: T25: T25: T25: T25: T25: T25: T25: T25 | 0 | Chloroform | | | | |
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| Mon Nitrobenzylakohol, G 2 i robenzylakohol, G 3 i robenzylakohol, G 4 i robenzylakohol, G 5 i robenzylakohol, G 5 i robenzylamin, 73 i Eig., Verh. 710; salz 73 : tertikres, Bi Nitrobenzylchlorid, 73 710. Nitrobenzyldichlorid, 73 710. Nitrobenzyldisulfid, 72 Nitrobenzyldisulfid, 73 robenzyldisulfid, 73 robenzyldisulfid, 73 robenzyldisulfid, 73 robenzylphenylamin salzs. 712; Eig. 713. Mon Nitrobenzylphenylamin salzs. 712; Eig. 713. | | Nie 11 1 - 1/Nie 1 - 11 1 - N | | | | |
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| Mon Nitrobenzylakohol, G trobenzylakohol, G trobenzylakohol, G trobenzylakohol, G trobenzylakohol, 78: Eig., Verb. 710; salz 10. Nitrobenzylakohol, G 28: tertikres, Bi 710. Nitrobenzylchlorid, 73: 710. Nitrobenzyldichlorid, 73: 710. Nitrobenzyldisulfid, 72: Nitrobenzyldisulfid, 73: 710. Nitrobenzylmercaptan, 65: 71: 65: 71: 71: 71: 71: 71: 71: 71: 71: 71: 71 | | sches, Bild., Eig. 327. | | | | |
| E trobenzylwasserstoff Mon ph Eig., Verh. 710; saln T3: tertifares, Bi Mon Mon Nitrobenzylchlorid, 73 710. Nitrobenzyldichlorid, 73 757. Mon Nitrobenzyldisulfid, 72 Nitrobenzylmercaptan, 65 Mon 66 Mon 67 Nitrobenzylphenylamin 68 Mon Nitrobenzylphenylamin 68 Nitrobenzylphenylamin 68 Nitrobenzylphenylamin 69 Nitrobenzylsphenylamin 69 Nitrobenzylsphenylamin 69 Nitrobenzylsphenylamin 69 Nitrobenzylsphenylamin 69 Nitrobenzylsphenylamin 69 Nitrobenzylsphenylamin | | 100 11 1 11 1 1 H # # 1 | | | | |
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| Eig., Verh. 710; salz 73: tertikres, Bi 710. Nitrobenzyldichlorid, 73: 357. Nitrobenzyldisulfid, 73: Mon 66: Sec. Nitrobenzylphenylamin salzs. 712; Eig. 713. Nitrobenzylsulfocyanid, Nitrobenzylsulfocyanid, Nitrobenzylsulfocyanid, | | 지 : : [[[[[[[[[[[[[[[[[| | | | |
| Mon Mon Nitrobenzylchlorid, 73 710. Nitrobenzyldichlorid, 73 757. Nitrobenzyldisulfid, 73 Nitrobenzylmercaptan, 652. Mon 66 652. Nitrobenzylphenylamin salzs. 712; Eig. 713 Mon Nitrobenzylsulfocyanid, | | Eig., Verb. 309. | | | | |
| Mon Nitrobenzylchlorid, 23 710. Nitrobenzyldichlorid, 2 357. Nitrobenzyldisulfid, 72 Nitrobenzylmercaptan, 652. Mon 65 652. Nitrobenzylphenylamin salzs. 712; Eig. 713. Mon Nitrobenzylsulfocyanid, | ild., Eig. 711. | Nitrochlormesitylen, 69 : Darst. 419. | | | | |
| Mon Nitrobenzyldichlorid, 2 357. Nitrobenzyldisulfid, 72 Nitrobenzylmercaptan, 6 652. Nitrobenzylphenylamin salzs. 712; Eig. 713 Mon Nitrobenzylsulfocyanid, | | Nitrochlornaphtaline, 76 : Verh. geg | | | | |
| 357. Nitrobensyldisulfid, 72 Nitrobensylmercaptan, 65 Mon Nitrobensylphenylamin salzs, 712; Eig. 713 Mon Nitrobensylsulfocyanid, | | Phosphorpentachlorid 408. | | | | |
| Mon Sitrobensyldisulfid, 72 Mon 66 652. Nitrobensylphenylamin 68 alrs. 712; Eig. 713 Mon Nitrobensylsulfocyanid, | Bild., Verh | Nitrochlorphenole, 70 : Const. 545; | | | | |
| Mon Nitrobensylmercaptan, 652. Nitrobensylphenylamin salzs. 712; Eig. 713 Mon Nitrobensylsulfocyanid, | a . Dild Vi- ere | Tt . Deset Via 440 | | | | |
| Mon 652. Nitrobenzylphenylamin 65 salzs. 712; Eig. 713. Mon Nitrobenzylsulfocyanid, | | Minochiorphenomanosaure, . A . Dir | | | | |
| Nitrobenzylphenylamin 65 salzs. 712; Eig. 713. Mon Nitrobenzylsulfocyanid, | · · · · · · · · · · · · · · · | SMEO TIA. | | | | |
| Mon Nitrobenzylsulfocyanid, | . 78 : Darst | 72 : Bild. 606 ; Kaliumsals 60 | | | | |
| Mon Nitrobenzylsulfocyanid, | | Nitrochlorphenoisullosauren, 44 : Bu | | | | |
| St Nitrobensylsulfos, Bary | | 711, 712; Eig., Salze, Verh. 712. | | | | |
| | | | | | | |
| 609. Nitrobenzylsulfos, Blei | eculting some second | benzol. Nitrochrysin, 78 : Bild. 862. | | | | |

Page 370:

Chlornitrobenzol, 71 : Bildungswärme 81; Verh. 431; 72 : Verh. 669, 670, 671; 74 : Darst. Eig. 372.

Chlornitrobenzol, $68:\alpha$, Darst. 348. Chlornitrobenzol, $68:\beta$, Darst. 344.

Page 544:

α- und β-Nitrochlorbenzol, 20 : Verh. 520.

Nitrochlorbenzole, 74: Siedep., Schmelzp. 361.

Page 546:

Monochlornitrobenzol (Nitrochlorphenyl), 62: Bild. 631.

Page 558:

Mononitrochlorbenzol, 75: Verh. 427.

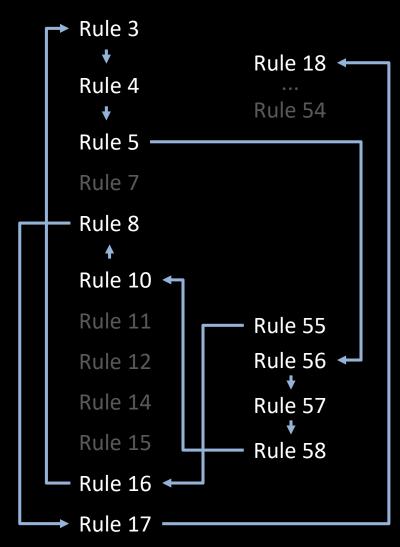
Jahresbericht über die Fortschritte der Chemie und verwandter Theile anderer Wissenschaften, Register zu den Berichten, 1867-1876 (Giessen: J. Ricker, 1880).

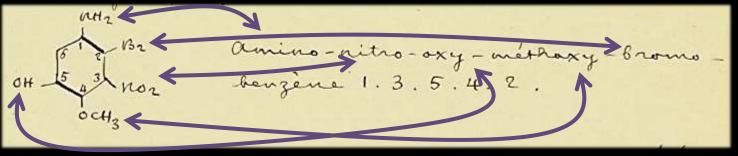
Geneva 1892: A chemical constitutional



moment

- "The official name of the compound is a faithful translation of its molecular constitution, representing the compound just as the structural formula does."
- Only applied to chemicals "of a known constitution" (the ones causing the nomenclature trouble)
- "Such systematic names... were really names of formulas rather than names of substances." – Alexander Crum Brown, pioneering user of structural formulas





The CHEMIST at WORK

XIV. MY WORK WITH CHEMICAL ABSTRACTS

JANET D. SCOTT

Journal of Chemical Education 15, no. 6 (1938): 271-75.



"Index workers" in Columbus, Ohio (1938)

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...

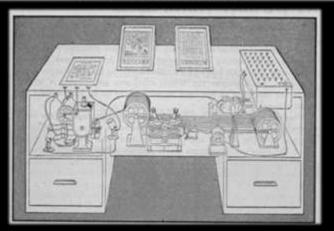


AS WE MAY THINK

IN WHICH MAN-MADE MACHINES WILL START TO THINK

by VANNEVAR BUSH

DIRECTOR OF THE OFFICE OF ECENTRIC RESEARCH AND DEVELOPMENT Condensed from the Atlantic Monthly, July 1945



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." (1947)

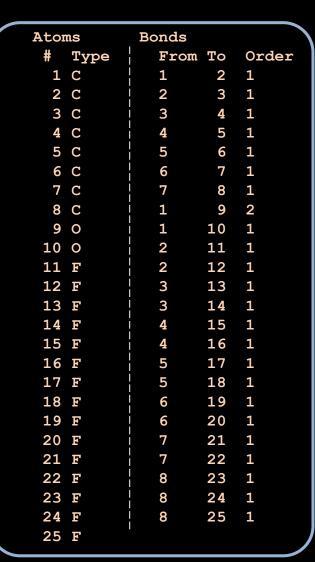
Calvin Mooers to Howard Mooers, 27 Jan 1947, Calvin and Charlotte Mooers Papers, Charles Babbage Institute Archives, University of Minnesota, CBI 81, Box 7, Folder 7.

Chemical
Abstracts
Service
Chemical
Substances
Registry

"CAS Registry"

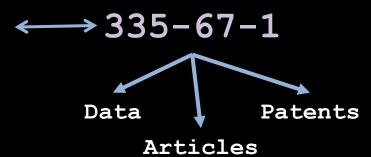
Think: "Fingerprint"

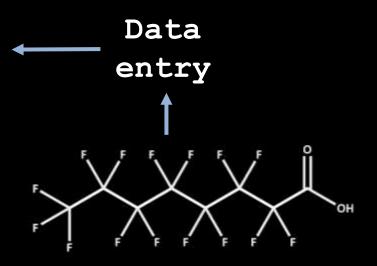
Connection Table

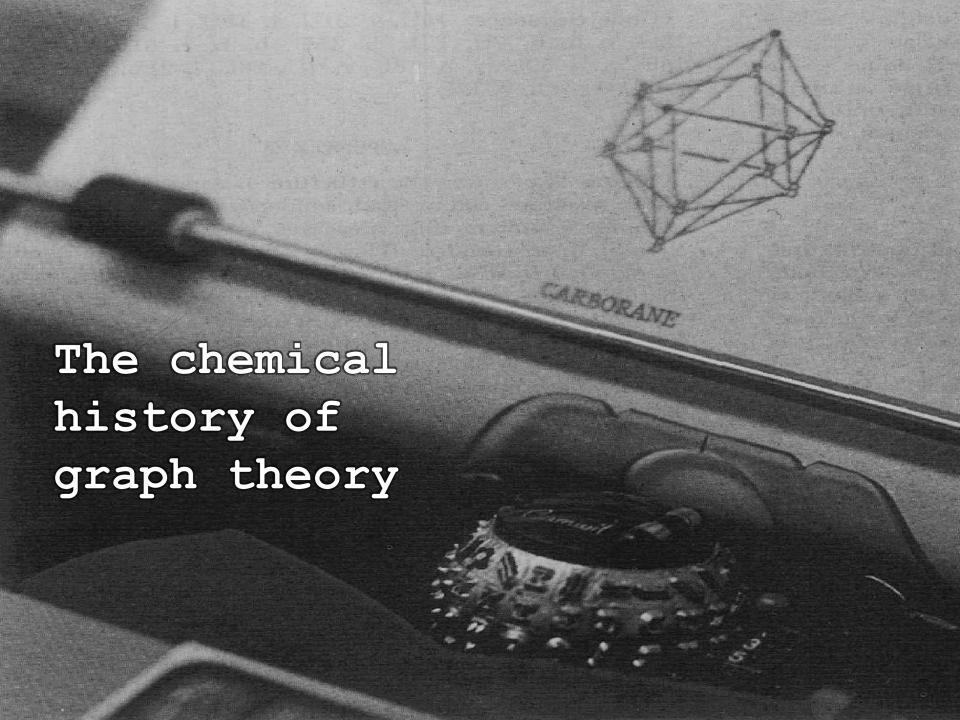


Think: social security number*

Registry Number







Cayley, *Phil. Mag.*, 1857. Same journal as Couper's structural formulas, one year prior. (Coincidence??)

this to the question in hand, PU consists of a single term repreFig. 1. Fig. 2. Fig. 3.

XXVIII. On the Theory of the Analytical Forms called Trees.

By A. CAYLEY, Esq.*

as above, of two terms (bis), viz. the first part cond part represents the 2 (bis) is at once formed

to be viewed as

to be viewed as

C...H²

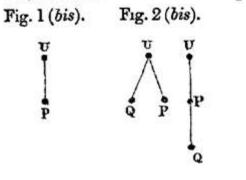
C...H²

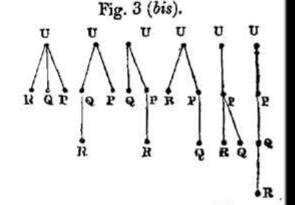
C...H²

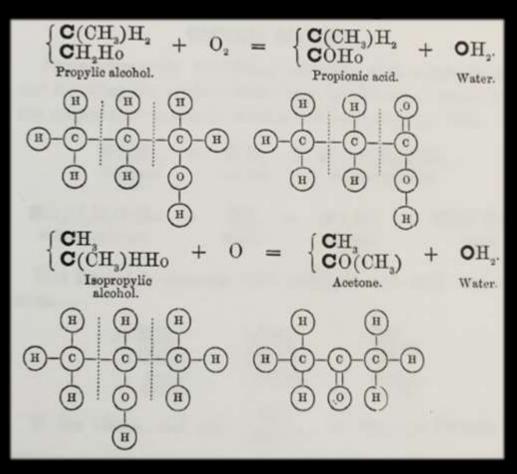
C...H³

these alcohols. The concomic of the

from the figure 1 (bis) by adding on a branch terminated by Q at each of the knots of the single part of fig. 1 (bis). In like manner RQPU consists of sixterms represented by the six parts of fig. 3 (bis),

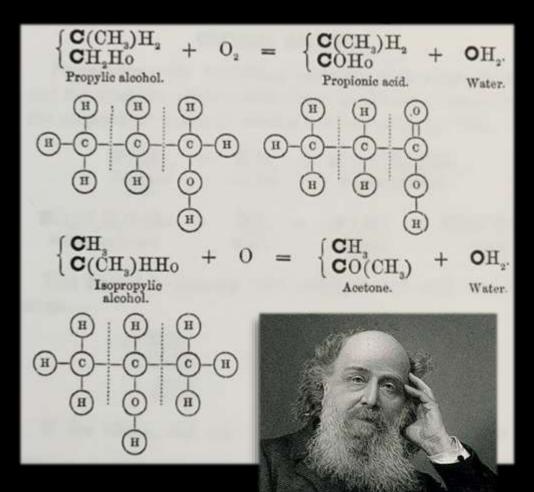






Frankland, Lecture Notes for Chemical Students (1866)

Inventing the "graph" as mathematical object



"Social individuals differ as egregiously as Isomers in their capacity for forming multifarious attachments."

"I feel as Aladdin might have done in walking in the garden where every tree was laden with precious stones."

<u>James Joseph Sylvester,</u> "On an Application of the New Atomic Theory," 1878.

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

Isomer-counting: fascinating to mathematicians and (some) chemists

"Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds" – Pólya's "enumeration theorem" (1937)

KOMBINATORISCHE ANZAHLBESTIMMUNGEN FÜR GRUPPEN, GRAPHEN UND CHEMISCHE VERBINDUNGEN.

VON

G. PÓLYA

[CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY, UNIVERSITY OF TEXAS]

THE NUMBER OF ISOMERIC HYDROCARBONS OF THE METHANE SERIES

By HENRY R. HENZE AND CHARLES M. BLAIR

RECEIVED MAY 11, 1931

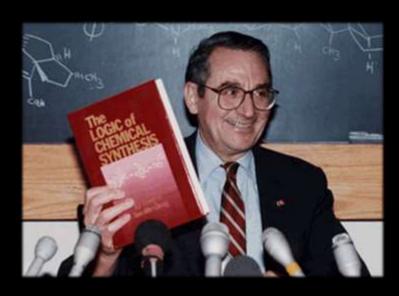
PUBLISHED AUGUST 5, 1931



LHASA

A COMPUTER PROGRAM
TO ASSIST IN THE DESIGN
OF SYNTHETIC ROUTES
TO COMPLEX
ORGANIC MOLECULES

Organic Synthesis



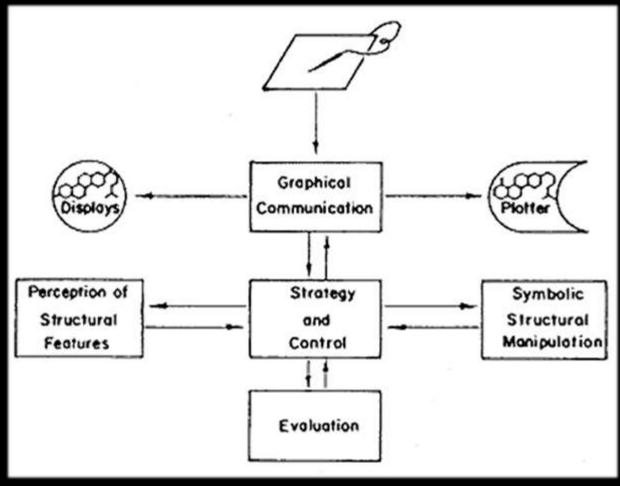
E. J. Corey (b. 1928)

Logic and Heuristics Applied to Synthetic Analysis: LHASA



E. J. Corey (b. 1928)

Corey & Wipke, "Computer-Assisted Design of Complex Organic Syntheses," Science (1969).



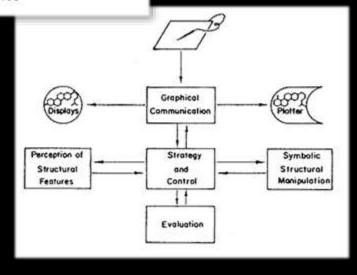
Retrosynthetic Analysis

VS.

- Direction of laboratory execution is 'synthetic'
- Represented as
 - —(s)
- Process is called a 'reaction'

- Direction of computer analysis is 'antithetic'
- 2. Represented as
- Process is called a 'transform'

"This organization, with its reversesynthetic or retrosynthetic focus, must be expressed explicitly and consistently in order to avoid intolerable confusion."



Corey et al., "Computer-Assisted Synthetic Analysis for Complex Molecules," *Journal of the American Chemical Society* (1972).

LHASA: Data structures

| 1U 1D 1S 5INFO | 4chg 3NBDS 3NATCH |
|----------------|-------------------|
| 9ATYPE | 9BOND1 |
| 9BOND 2 | 9BOND3 |
| 9BOND4 | 9 BOND 5 |

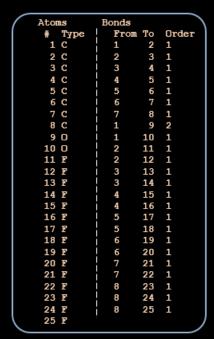
| ¹ U ¹ D ⁹ BIN | FO | ³ BSTEREO | ⁴ BTYPE |
|--|----|----------------------|--------------------|
| 9 _{ATOM1} | | ATOM 2 | |

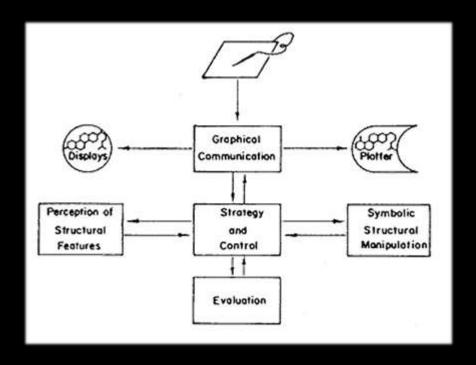
Fig. 7 (left). The structure of an atom table entry.

Fig. 8 (above). The structure of a bond table entry.

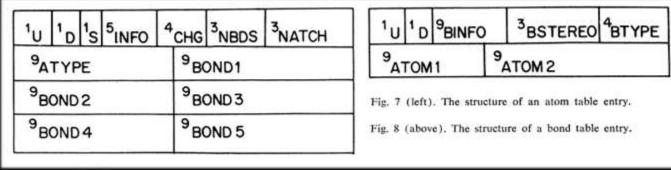
Corey & Wipke (1969).

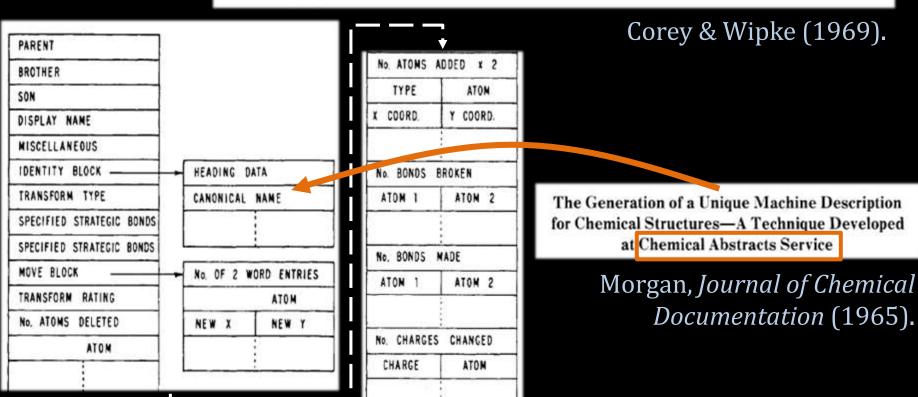
Connection Table





LHASA: Data structures





Corey et al., "Computer-Assisted Synthetic Analysis for Complex Molecules," *Journal of the American Chemical Society* (1972).

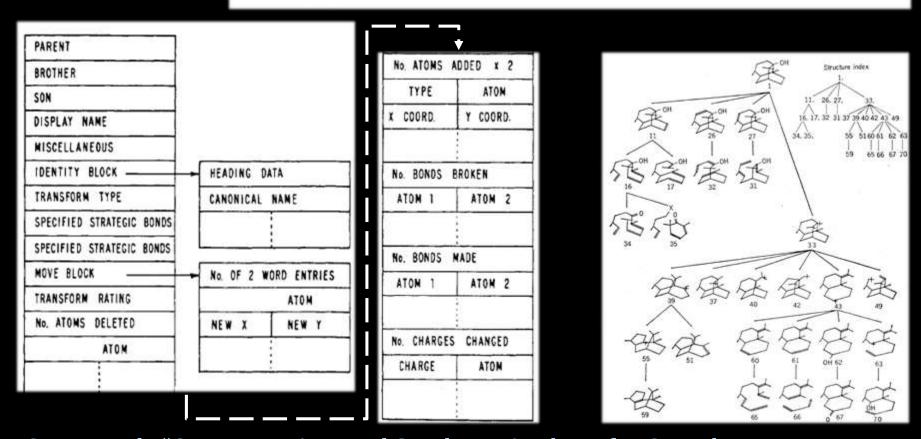
LHASA: Data structures

| 1 _U 1 _D 1 _S 5 _{INFO} | 4chg 3NBDS 3NATCH |
|--|-------------------|
| 9ATYPE | 9BOND1 |
| 9BOND 2 | 9BOND3 |
| 9BOND 4 | 9 BOND 5 |

| ¹u ¹ | D | 9 _{BINFO} | ³ BSTEREO | ⁴ BTYPE |
|-----------------|----|--------------------|----------------------|--------------------|
| 9 _{AT} | ОМ | 1 | 9 ATOM 2 | |

Fig. 7 (left). The structure of an atom table entry.

Fig. 8 (above). The structure of a bond table entry.



Corey et al., "Computer-Assisted Synthetic Analysis for Complex Molecules," *Journal of the American Chemical Society* (1972).

LHASA as chemistry rather than computing

"No 'programming' is involved, since the <u>interpretive</u> table language permits rapid

...THIS SUBROUTINE IS CALLED TO CLEAR AWAY ANY UNDESIRABLE FUNCTIONALITY
...ALPHA TO A KETONE ON THE RING

ALPHCHK IF NO HYDROGEN ON THE SPECIFIED ATOM THEN GO TO 19

IF THERE IS NOT A WITHDRAWING GROUP ON THE SPECIFIED ATOM THEN GO TO 18

IF THE SPECIFIED ATOM IS THE SAME AS CARBON*2 THEN RETURN SUCCESS
IF BOND*5 IS A FUSION*BOND THEN RETURN SUCCESS
IF THERE IS NOT A NITRO ON THE SPECIFIED ATOM THEN GO TO 18

EXCHANGE THE GROUP FOR AN AMINE

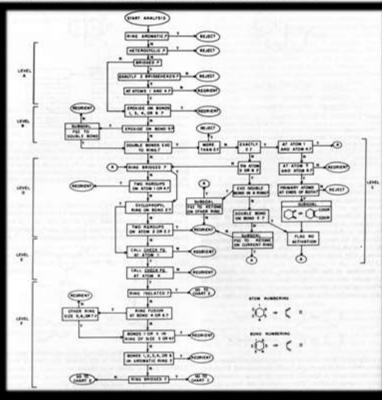
IF SUCCESSFUL THEN GO TO J2 OTHERWISE RETURN FAIL

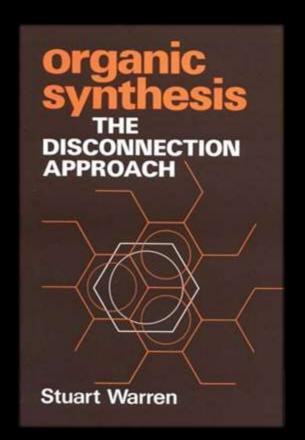
18

IF THERE IS A HALIDE ON THE SPECIFIED ATOM THEN GO TO J2
IF THERE IS A WITHDRAWING GROUP ON THE SPECIFIED ATOM THEN GO TO J2

and direct transcription of the <u>information contained in the flow</u> <u>charts</u> into a form that is "readable" by the computer."

"Such undertakings are not less challenging and rewarding than the conception and execution of a specific synthesis." (Corey et al. 1974).



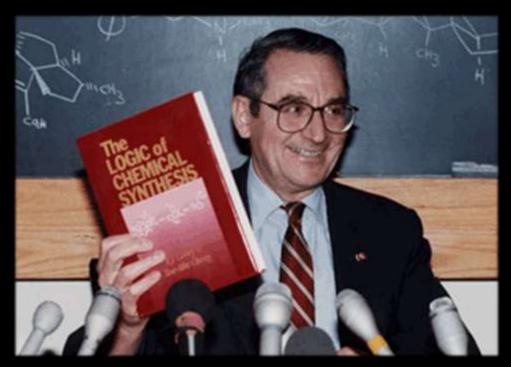


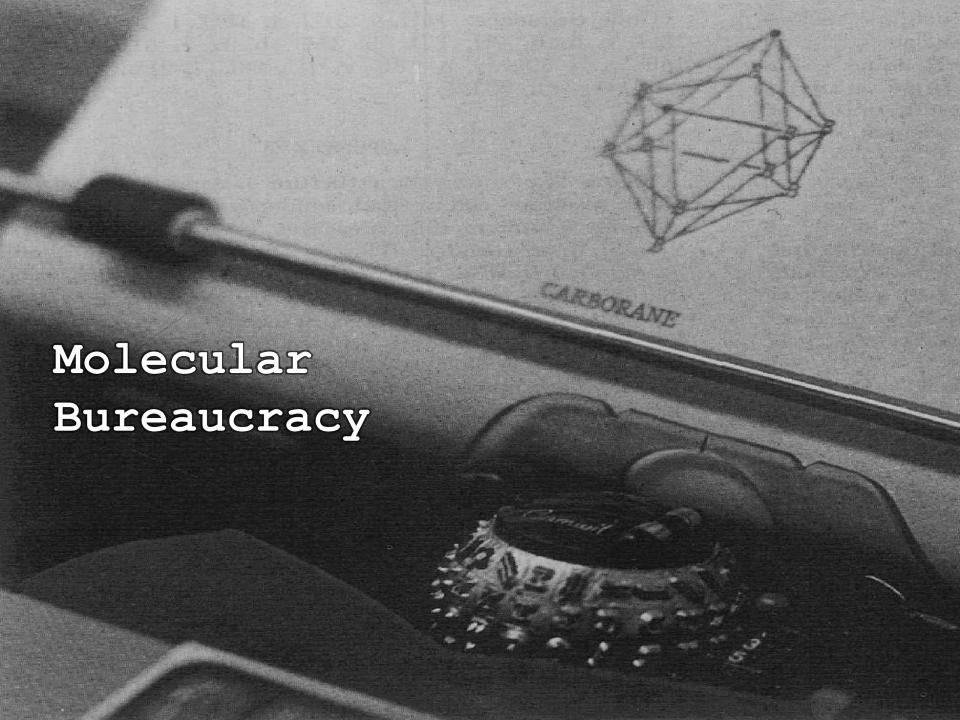
1982

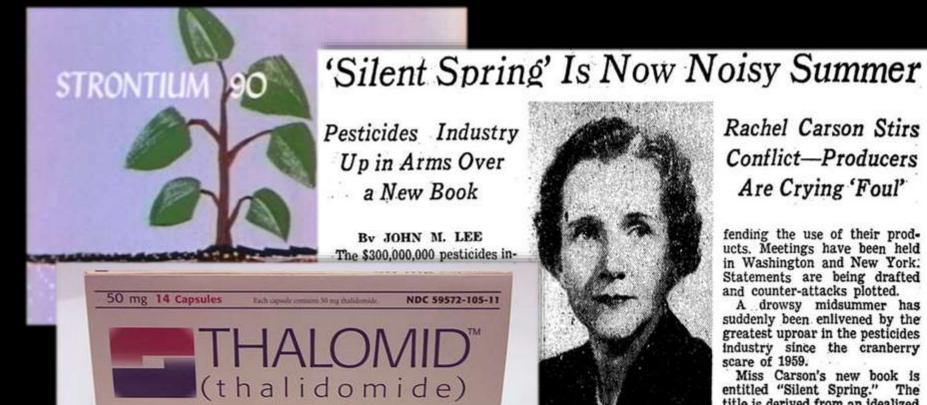
"The aim of this book is to show you how this planning is done: to help you learn the disconnection approach to organic synthesis."

"The interactive program, LHASA... is designed to emulate the problem solving techniques used by chemists. In turn, the LHASA project has been of great value in the development of new and general ways of thinking about synthesis."

1989







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.

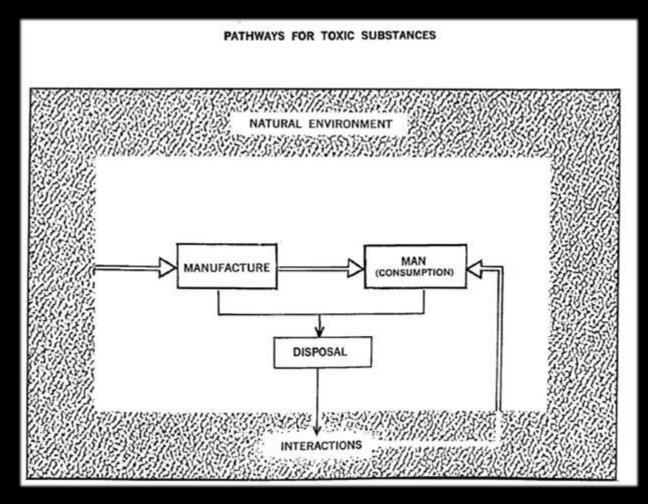
Miss Carson's new book is entitled "Silent Spring." title is derived from an idealized situation in which Miss Carson envisions an imaginary town

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

SMOKING and HEALTH

REPORT OF THE ADVISORY COMMITTEE TO THE SURGEON GENERAL OF THE PUBLIC HEALTH SERVICE

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."

CAS to Study Registry of Chemical Compounds

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

The CAS Registry Number: interface for assembling "a much more coordinated and more complete computer-based file of toxicological information," constituting a "total body of chemical and biological information"



Donald F. Hornig A critical experiment

(1965)

Connection Table

| Atoms | Bonds | |
|----------------------|--------------------------------------|-------|
| # Type | From To | Order |
| 1 0 | 1 2 | 1 |
| 2 C | 2 3 | 1 |
| | 3 4 | 1 |
| 4 C | 4 5 5 6 | 1 |
| | | 1 |
| | 6 7 | 1 |
| , . | 7 8 | 1 |
| 8 C | 1 9 | 2 |
| 9 🛭 | 1 10 | 1 |
| 10 0 | 1 10 2 11 2 12 | 1 |
| 11 F | 2 12 | 1 |
| 12 F | 3 13 | 1 |
| | 3 14 | 1 |
| 14 F | 4 15 | 1 |
| 14 F 15 F 16 F | 4 16 | 1 |
| | | 1 |
| 17 F | 5 18 | 1 |
| 18 F | 6 19 | 1 |
| 19 F | 6 20 | 1 |
| 20 F | 5 18 6 19 6 20 7 21 7 22 | 1 |
| 21 F | 7 22 | 1 |
| 22 F | 8 23 | 1 |
| 23 F | 8 24 | 1 |
| 24 F | | 1 |
| 25 F | | |

√335-67-1



NATIONAL CANCER INSTITUTE



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."



Toxic Substances

Toxic Substances Control Act Chemical Substance Inventory

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

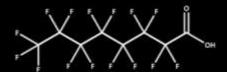
Frederick H. Siff, "Inventory Information in the Chemical Abstract Service," in 2^{nd} Annual ADP Conference (Washington: EPA, 1977), H-11.

"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."

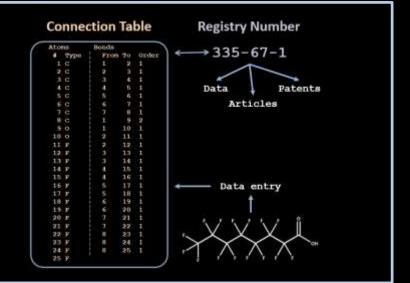
Steven Jellinek, head of EPA Office of Toxic Substances, 1977-1981 (in 2010)

Molecular Bureaucracy





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

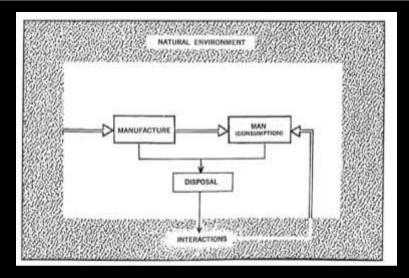














shared knowledge shared progress

SEARCH

PRODUCTS NEWS LIBRARY MEMBERSHIP INITIATIVES **EVENTS** MEMBERS KAPTIS DEREK NEXUS **EFFIRIS** METEOR NEXUS MIRABILIS SARAH NEXUS SETARIA VITIC ZENETH ABOUT LHASA



















Some arguments

- The molecular ideal originated as a way to organize printed chemical bibliographies, mostly in order to support chemical industry R&D
- It (purposefully!) did not address all sorts of materials & ways of thinking about materials important to chemists
- It had historically-grounded affinities with mechanical methods for information retrieval
- Mechanizing compilation of chemical reference books

 → chemical databases that presumed/suggested the
 universality of the molecular ideal → computational
 methods, information infrastructures, and
 administrative procedures that took the molecular ideal
 for granted and/or built on it ("molecular bureaucracy")

There's the story, then there's the real story, then there's the story of how the story came to be told. Then there's what you leave out of the story. Which is part of the story too.

Margaret Atwood, MaddAddam (2013)

(Being) Digital questions

- Relationship with informatics and data science more broadly?
- Can chemical/materials Firms
 data (& web ontologies!)
 reflect multiple &
 relational ontologies?

For:
historians
data sci's
designers
softwaredevelopers
chemists
activists

(Being) Material questions

- Relationship with chem.
 engineering, process
 control & finance (esp. in
 petrochemicals)?
- What if we take all substances as nonmolecular? (Nanomat'ls!)
- How to work with, against, & beyond molecular bureaucracy?
 What would a <u>desire-based</u>, not <u>damage-based</u> chemical data regime look like? (Eve Tuck, "Suspending Damage," 2009)
- Can chemical substances be enacted as situated, history-laden objects-in-relation, not abstract & interchangeable?

"Remapping Chemicals, Environments, and Toxicity"

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

Charles Gerhardt, 1850

