The machine and the molecule
Chemistry in
the history of AI

Evan Hepler-Smith

Boston College

heplers@bc.edu/evanheplersmith.com

"Historical epistemology and attention to practice have long been central concerns for historians of science"

1. **Situating "universal" knowledge in specific places, rhetorics, practices**

2. **Attending to more activities, people, and places *qua* knowledge-making**

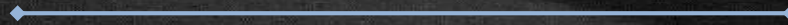3. **Including (perhaps starting from!) histories of *applied* science**

my talk today

The histories of computing(s)

MICHAEL S. MAHONEY

Mahoney says: figure out how "various communities of computing...have (re)shaped not only their own practice, but also computers and their adaptation by others" (2005).

This may be one productive approach to history of AI.

But what's a "community of AI" (or a community of computing, for that matter)? How do you circumscribe it?

One answer: look for <u>knowledge communities</u> and their <u>attractors</u>, following Ann Johnson (*Hitting the Brakes*, 2009).

THE DRUG-MAKER'S GUIDE TO THE GALAXY

SCANNING SPACE ...

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 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 books and good reference literature**" (1919)

"[T]he Beilstein Handbook has always been basically **a 'computerized' collection waiting for the suitable computerized handling system to be discovered**" (2003)

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

Joshua Lederberg

APPLICATIONS OF ARTIFICIAL INTELLIGENCE FOR ORGANIC CHEMISTRY

The DENDRAL Project

Ed Feigenbaum (expert systems AI)

DENDRAL (1964-1980ish)

"THE PROSPECTS FOR AUTOMATIC SCIENCE

"DENDRAL illustrates the state of the art in automatic hypothesis formation."

Chemico-Linguistics: Computer Translation of Chemical Nomenclature
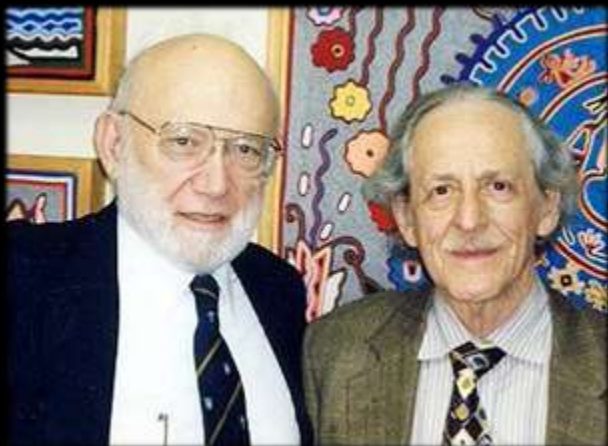
Eugene Garfield

Joshua Lederberg

"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" (Garfield 1961)

APPLICATIONS OF ARTIFICIAL INTELLIGENCE FOR ORGANIC CHEMISTRY

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DENDRAL

(1964-1980ish)

"It is the ultimate objective of this work to generate accurate molecular formulas for all chemical names and also to display and print ideographs, that is, structural diagrams" (Garfield 1961)

"DENDRAL-64... outlines an approach to formal representation of chemical graph structures. ...This was the essential prerequisite for an AI program." (Lederberg 1987)

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
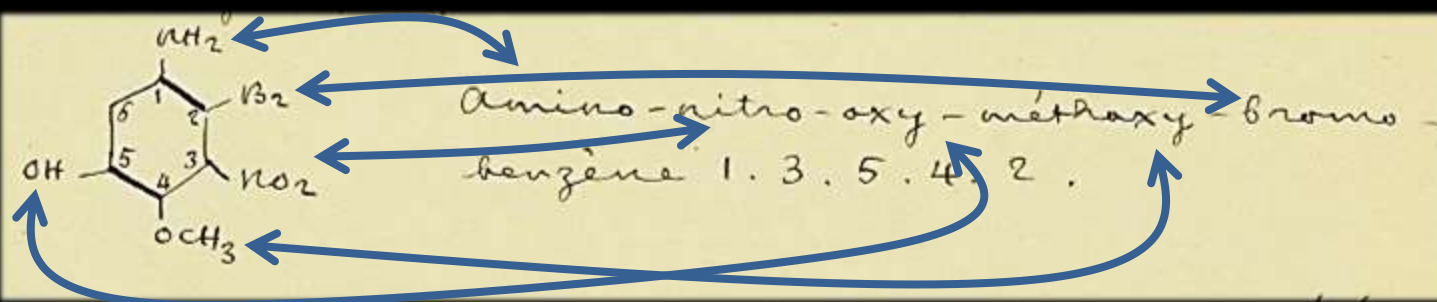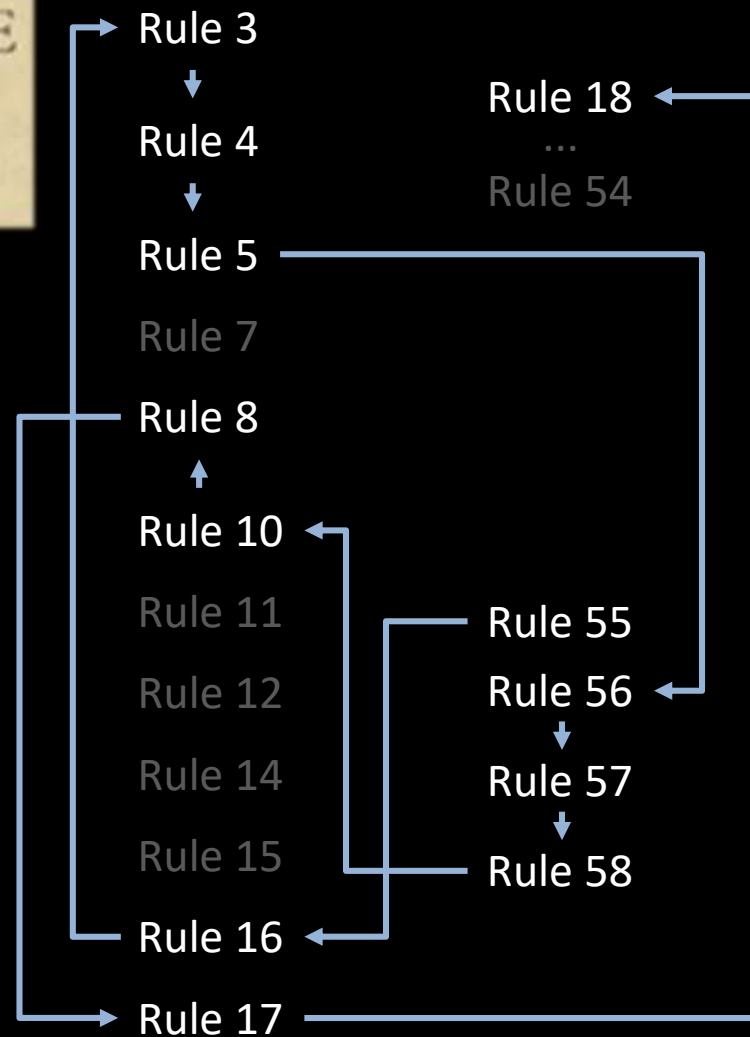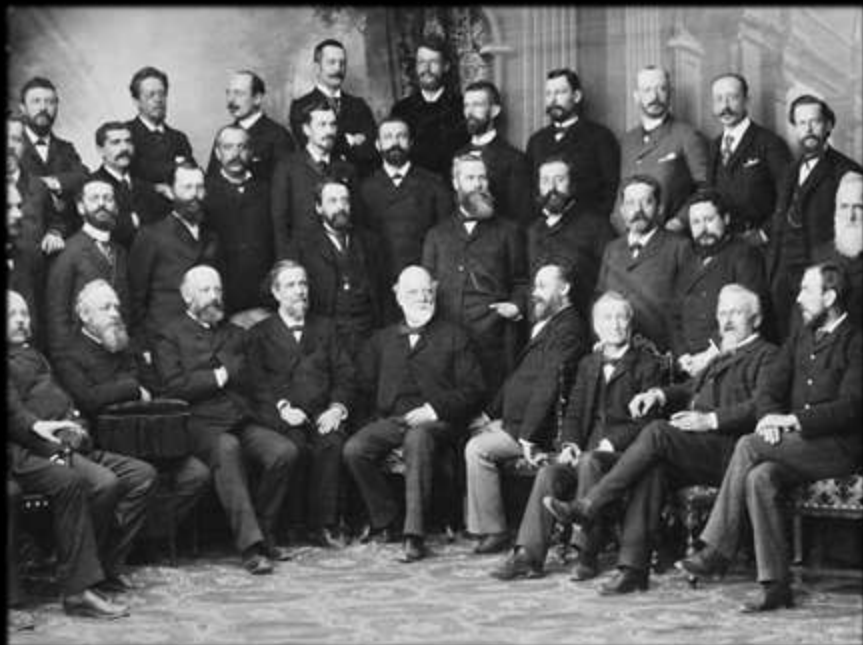
STUDIENGRUPPE FÜR SYSTEMFORSCHUNG

Gertrud Hornke
' '

Maschinelle Dokumentation
in der organischen Chemie

These: 1960s
Others: 1940s
to present

COMMISSION INTERNATIONALE
POUR LA RÉFORME DE LA NOMENCLATURE CHIMIQUE
réunie à Genève du 19 au 22 avril 1892

Rule 3
Rule 4
Rule 5
Rule 7
Rule 8
Rule 10
Rule 11
Rule 12
Rule 14
Rule 15
Rule 16
Rule 17

Rule 18
…
Rule 54
Rule 55
Rule 56
Rule 57
Rule 58

Amino-nitro-oxy-méthoxy-bromo-benzène 1.3.5.4.2.

1892

Chemico-Linguistics: Computer Translation of Chemical Nomenclature

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Scrutinizing these "applications" of AI in chemistry leads us to a _**knowledge community**_ centered on the attractor of formal representation of molecular structure, enabling mappings of diagrams to names to machine notations.

Chemico-Linguistics: Computer Translation of Chemical Nomenclature

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Scrutinizing these "applications" of AI in chemistry leads us to a _**knowledge community**_ centered on the _attractor_ of formal representation of molecular structure, enabling mappings of diagrams to names to machine notations.

Note that chemical communities of AI(s) were working with data (including linguistic data) _known to be_ configured according to a structured, interpretable data model—"a 'computerized' collection waiting for the suitable computerized handling system to be discovered." Chemistry (and other domains?) seemed to demand "first culture" (Breiman) approaches to AI and thus provided a concrete, practical justification for pursuit of such approaches.

Logic and Heuristics Applied to Synthetic Analysis: LHASA (1967-)
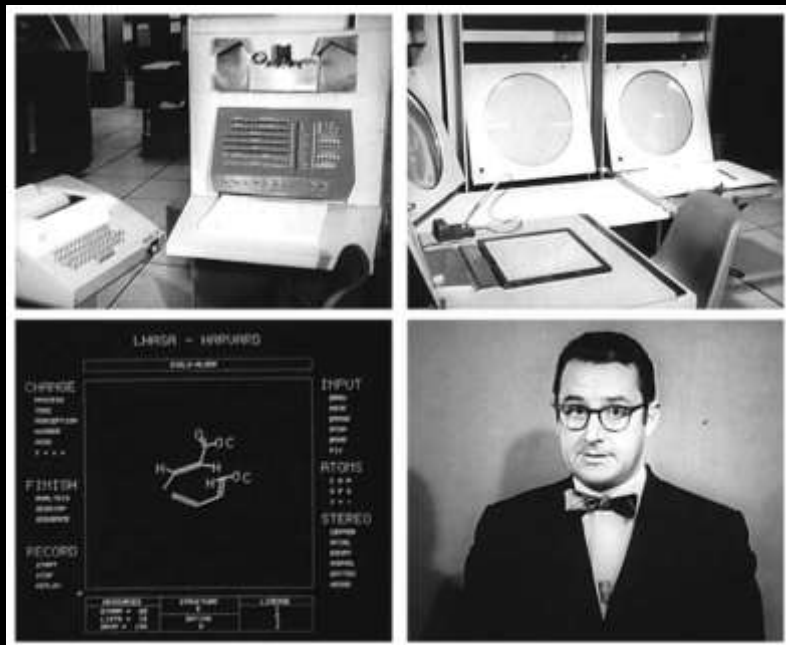
Explication: applied AI as method-making for __non-artificial__ experts, such that the method can be understood as formalizing and extending expert intuition.
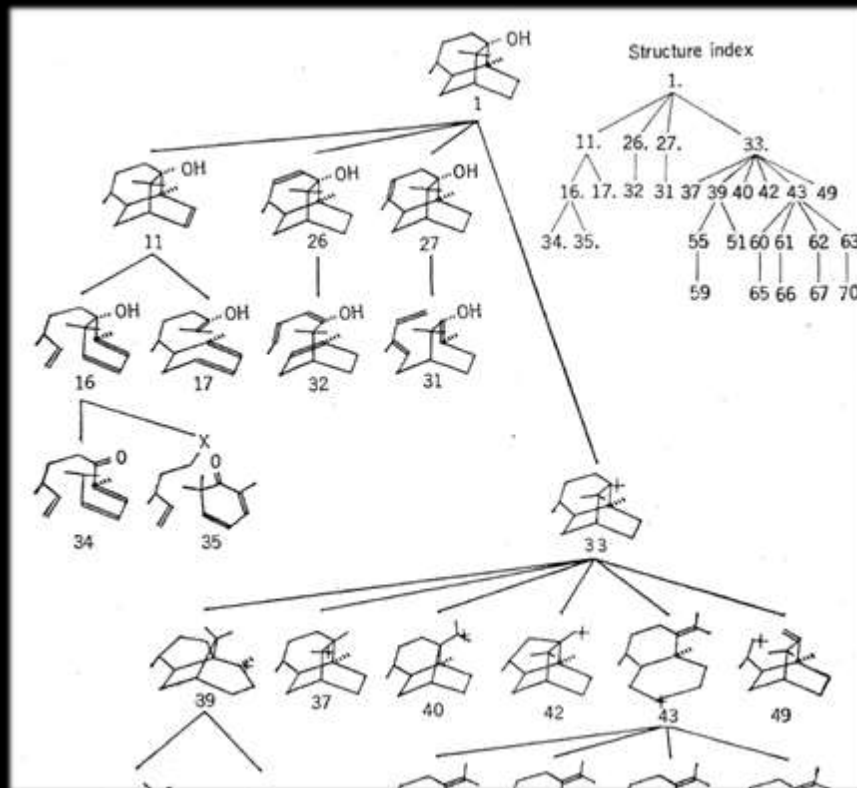
"The interactive program, LHASA... is designed to __emulate the problem solving techniques used by chemists__. In turn, the LHASA project has been of great value in the __development of new and general ways of thinking about synthesis__" (Corey 1988).

Non sequitur that isn't really a non sequitur:

There is an ethical imperative to pluralizing histories of AI(s) in this way—that is, looking to communities of (applied) AI.

Making Kin with the Machines
by Jason Edward Lewis, Noelani Arista, Archer Pechawis, and Suzanne Kite
Jul 16, 2018

Essay Competition Winner

"Digital Natives":
How Medical and Indigenous
Histories Matter for Big Data

by Joanna Radin*

"I am not worried about rogue hyper-intelligences going Skynet to destroy humanity. I am worried about anonymous hyper-intelligences working for governments and corporations, implementing far-reaching social, economic, and military strategies based on the same values that have fostered genocide against Indigenous people worldwide and brought us all to the brink of environmental collapse."

"A problematic aspect of the current AI debate is the assumption that AIs would be homogeneous.... The country to which AI currently belongs [figuratively, but maybe more than figuratively? -EHS] excludes the multiplicity of epistemologies and ontologies that exist in the world."

"I am not making an argument about which entities qualify as relations, or display enough intelligence to deserve relationships. By turning to Lakota ontology, these questions become irrelevant. Instead, Indigenous ontologies ask us to take the world as the interconnected whole that it is, where the ontological status of non-humans is not inferior to that of humans....To approach this relationship ethically, we must reconsider the ontological status of each of the parts which contribute to AI, all the way back to the mines..."

Making Kin with the Machines
by Jason Edward Lewis, Noelani Arista, Archer Pechawis, Suzanne Kite

… "we must reconsider the ontological status of each of the parts which contribute to AI…"
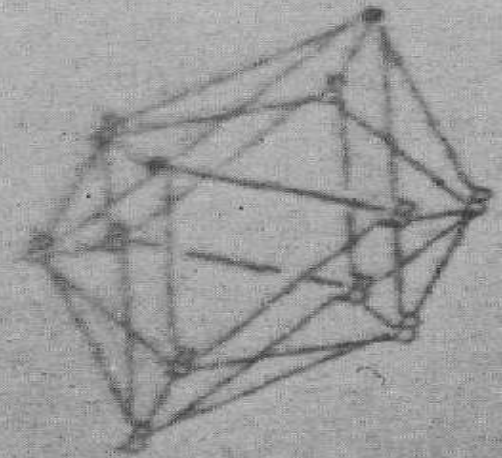
Thank you!

Evan Hepler-Smith

heplers@bc.edu

evanheplersmith.com

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