

Chapter 15. The Dendral Project

The Quest for Artificial Intelligence, Nilsson, N. J., 2009.

Lecture Notes on Artificial Intelligence, Spring 2012

Summarized by Lee, Bado and Seok, Ho-Sik

Biointelligence Laboratory
School of Computer Science and Engineering
Seoul National University

Contents

Collaborators of Dendral Project

Collaborators of Dendral Project

Discerning the structure of chemical compound

Task and Method

What is Dendral Project

Dendral Project

Dendral

Dendral Rule

Dendral Rule

Importance of The Dendral Project

Importance of The Dendral Project

Overview of Chapter 15

- Collaborators of Dendral Project
 - Edward Reigenbaum, Joshua Lederberg, Bruce Buchanan
- The application of Dendral Project
 - Discerning the structure of chemical compound
- What is Dendral Project?
 - Use of expert knowledge
 - Dendral Algorithm
 - Dendral Rule
- Importance of The Dendral Project

Collaborators of Dendral Project

■ Edward Reigenbaum

- “Creating models of the thinking processes of scientists, especially the processes of empirical induction by which hypotheses and theories were inferred from data”
- “What I needed was a specific task environment in which to study these issues concretely”

■ Joshua Lederberg (1925-2008)

- A Nobel Prize-winning geneticist and founder of the Stanford Department of Genetics
- Discerning the structure of a chemical compound from knowledge of its atomic constituents and from its mass spectrogram

- Edward found Joshua and they soon collaborated. Bruce Buchanan (1940-) joined in 1966.

Collaborators of Dendral Project

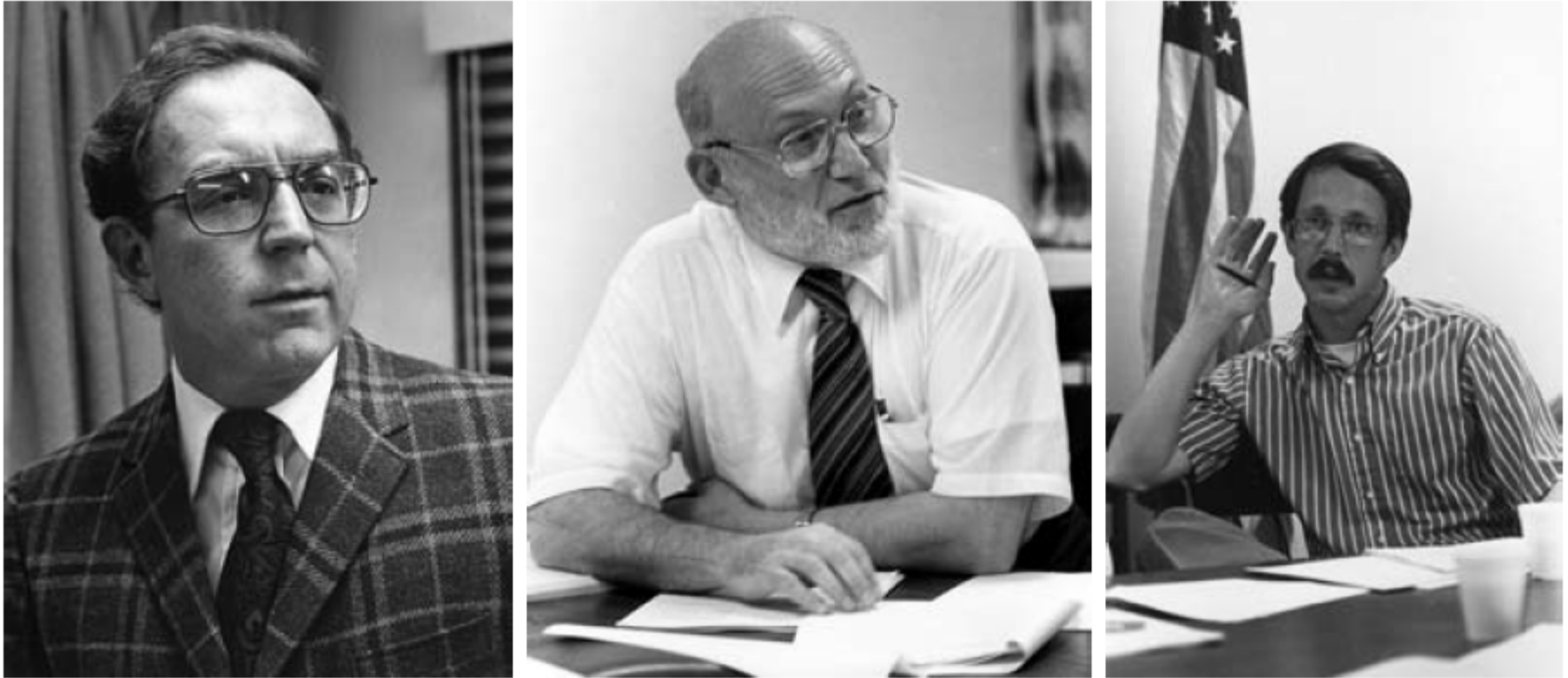


Figure 15.1: Edward Feigenbaum (left), Joshua Lederberg (middle), and Bruce Buchanan (right). (Photographs courtesy of Edward Feigenbaum.)

Discerning the structure of chemical compound

■ Task

- The atoms composing a molecule are arranged in a geometric structure, as Figure 15.2 and chemists want to know what that structure is.

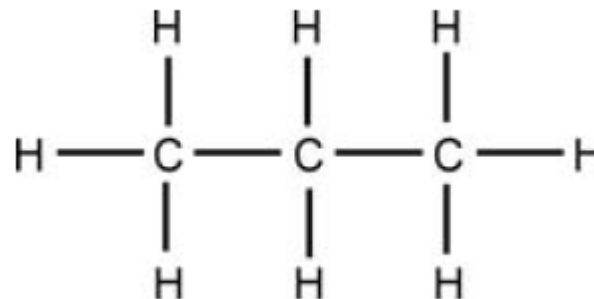


Figure 15.2: The structure of the propane molecule.

■ Method

- An experienced chemist uses “accumulated knowledge” about how compounds tend to break up in the mass spectrometer (Figure 15.3) to make good guesses about a compound’s structure.

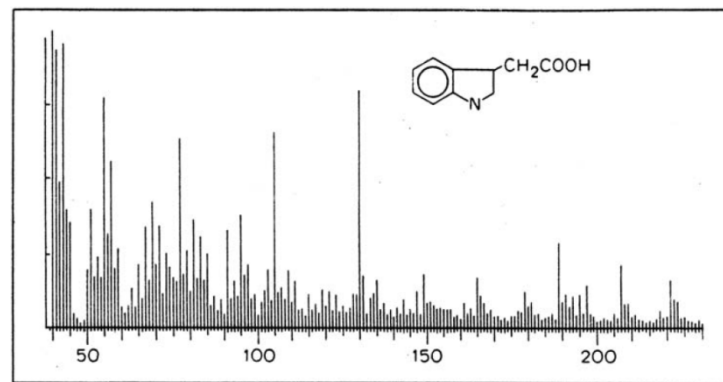


Figure 15.3: A mass spectorgram.

What is Dendral Project?

■ Dendral Project

- Attempting to construct computer programs that could use mass spectorogram data, together with the chemical formula of a compound, to “elucidate” the structure of the compound.

■ Dendral

- Computer procedure (an acronym for Dendritic Algorithm) that could generate all topologically possible acyclic structures given the chemical formula and other basic chemical information about how atoms attach to other atoms.

Dendral Rule

■ Dendral Rule

- This knowledge could be used to limit the possible structures generated by Lederberg's Dendral algorithm

One example of a Dendral rule:

IF The spectrum for the molecule has two peaks
 at masses X_1 and X_2 such that:

$$X_1 + X_2 = M + 28$$

and

$X_1 - 28$ is a high peak

and

$X_2 - 28$ is a high peak

and

at least one of X_1 or X_2 is high

Then The molecule contains a ketone group

Importance of The Dendral Project

- “Knowledge-is-power” hypothesis
 - We must hypothesize from our experience to date that the problem solving power exhibited in an intelligent agent's performance is primarily a consequence of the specialist's knowledge employed by the agent, and only very secondarily related to the generality and power of the inference method employed. Our agents must be knowledge-rich, even if they are methods-poor.
- Embedding the knowledge of experts in AI programs led to the development of many “expert systems“
- Also led to increased concentration on specific and highly constrained problems and away from focusing on the general mechanisms of intelligence