The Chemical Table: An Open Dialog between Visualization and Design

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Chemical Table

- Created over 300 years ago
- Tool to organize and visualize chemical reactivity
- Evolved into periodic charts and tables
- During the past 150 years over 700 visualizations of chemical periodicity have appeared

Chemical Tables and Charts

- Organizing constructs for basic components of chemical knowledge
- Search for complete, coherent, systematic representation of chemical information organization
- two-dimensional periodic table remains *de facto* representation

Chemical Tables and Charts

Contents: chemical information

- e.g. atomic weights, ionization potentials, oxidation states, reaction rates, melting points, crystal structures
- Physically measurable quantities
 - But have neither intrinsic nor causal geometric correlations

Must be considered a visualization of abstract data organized on a conceptual substrate such as a xy grid.

Chemical Tables and Charts

designed artifacts
built to organize chemical knowledge
Used as tools for reasoning
dynamic as well
form is *plastic*

Purpose of Talk

- Review the chemical table from an historical perspective as a designed tool for information visualization
- Argue why the 2D Periodic Table is the *de facto* representation of chemical information

Representations

TablesChartsPhysical Models

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Étiénne-François Geoffroy's "Table des différents rapports, 1718

Dimitri Mendeleev's periodic table of 1869



Charles Janet's periodic table of 1927



Contemporary Periodic Table by U.S. NIST



Bayley-Thomsen-Bohr Periodic Table of 1882, 1895, 1922, & 1989



Periodic Spiral by Electric Prism, Inc.





Alexandre-Émile Béguyer de Chancourtois's Telluric Screw, 1862. ©Science Museum, London. Used with permission.

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Gustavus Detlef Hinrichs's spiral/radial alignment, 1867



Theodor Benfey's spiral table of 1960.



Georg Schaltenbrand's helices of 1920



William Crooke's *pretzel* model of 1888. ©Science Museum, London. Used with permission.



Roy Alexander's contemporary periodic model based on Courtines and Clark's model of 1925

Analysis

- Complex three dimensional charts and physical models are:
 - difficult to construct
 - even more difficult to interpret without machine intervention
- Advances in CG and HCI not used to build systems that display these complex relationships



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Tables

- important data visualization tool
- first stage in information visualization pipeline
- compactly organized structure
- facilitates understanding of relationships among different data

Four Rationales for Table Usage

- Exploration
- Communication
- Storage
- Illustration

H. Wainer, *Educational Researcher*, 21(1) 1992, pp. 12-23.
H. Wainer, *Journal of Educational and Behavioral Statistics*, Spring 1997, 22 (1) pp. 1-30.

Analysis of Geoffroy's Table Usage

Table explored

- Used to find best reaction to solve laboratory separation problems
- Communication medium
 - translated chemical narrative of reaction selection into understandable graphic form
- Open-ended storage medium
 - contained a history of chemical practice that could be appended to over time
- an *illustration* serving the greater narrative of chemical synthesis

acted as a focal point for analysis and discourse

Requirements for Table Design

- Must reflect kinds of questions asked of the data it contains.
- Three levels of inquiry:
 - 1. Elementary questions about data:
 - single category data inspection or extraction
 - 2. Intermediate questions about data:
 - comparisons, trends, and relationships among data entries
 - 3. General questions about data:
 - require understanding of the underlying data structure and the ability to build a level of abstraction for the entire data set

Analysis of Modern Table Design

Single category data inspection :

each location is a box, a container that displays atomic data.

Comparisons and relationships :

- Designed to organize chemical information so that relationships among chemical properties may be exposed
- Understanding of the data structure :
 - chemical table continued design and redesign

Requirements for Tool Design

Direct access to data

- Accurate encoding of information
- Easy integration into work practice
- Short learning curve





Further requirements for Hypermedia Tables

Ability to display meaningful patterns trends, and exceptions
 Use of visualization best practices
 Dynamic linking of table contents to supporting chemical documentation and narrative

Summary & Conclusions

- Explored the historical development of the chemical table as a tool designed for chemical information visualization
- Shown why the design of the twodimensional periodic table remains the *de facto* standard for chemical information display
- Periodic Table is dynamic and continues to evolve



Suzanne Caporael, *Periodic Table of the Elements*, 1995. 112 books, oil on linen, muslin, 78" x 192"

Thank you !