The Chemical Table: An Open Dialog between Visualization and Design

Francis T. Marchese
Department of Computer Science
Pace University
New York, NY 10038

http://csis.pace.edu/~marchese
fmarchese@pace.edu

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

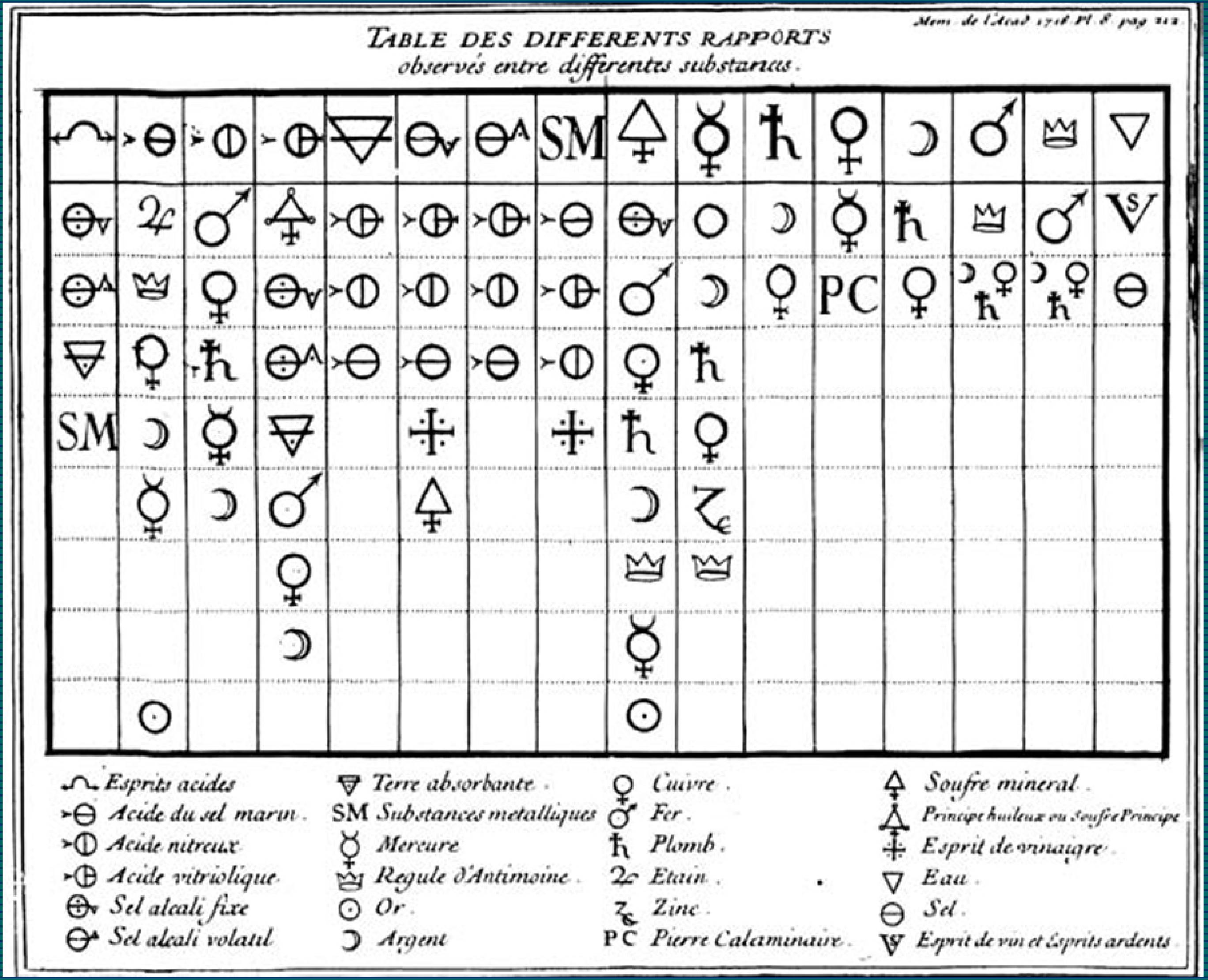
- designed artifacts
- built to organize chemical knowledge
- Used as tools for reasoning
- dynamic as well
- form is *plastic*

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

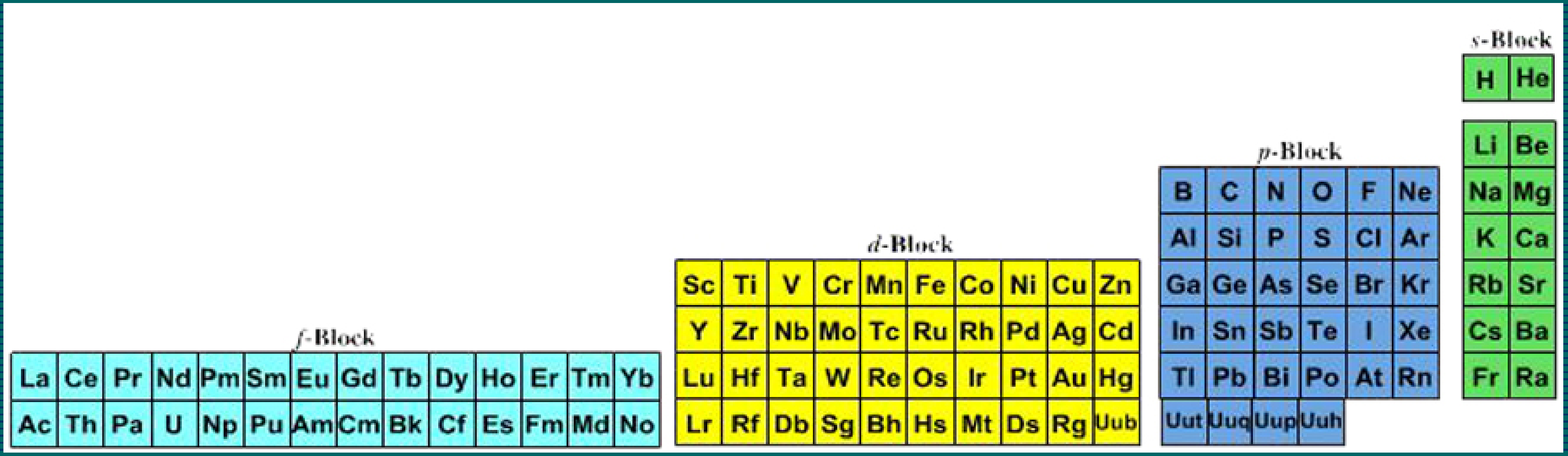
- Tables
- Charts
- Physical Models



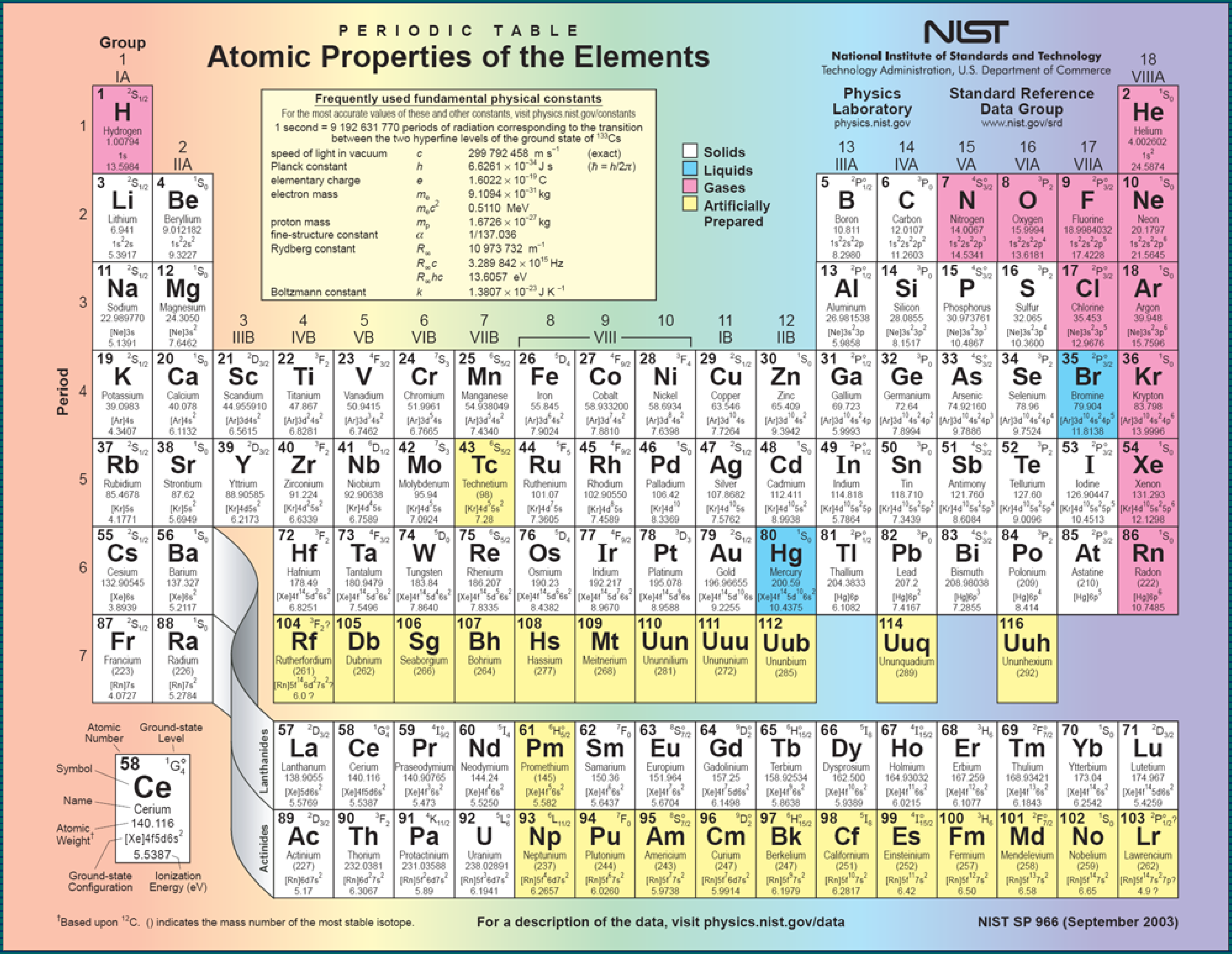
Étiénne-François Geoffroy's "Table des différents rapports, 1718

			Ti=50	Zr=90	?=180.
			V=51	Nb=94	Ta=182.
			Cr=52	Mo=96	W=186.
			Mn=55	Rh=104,4	Pt=197,4.
			Fe=56	Rn=104,4	Ir=198.
			Ni=Co=59	Pl=106,6	O-=199.
H=1			Cu=63,4	Ag=108	Hg=200.
	Be=9,4	Mg=24	Zn=65,2	Cd=112	
	B=11	Al=27,4	?=68	Ur=116	Au=197?
	C=12	Si=28	?=70	Sn=118	
	N=14	P=31	As=75	Sb=122	Bi=210?
	O=16	S=32	Se=79,4	Te=128?	
	F=19	Cl=35,5	Br=80	I=127	
Li=7	Na=23	K=39	Rb=85,4	Cs=133	Tl=204.
		Ca=40	Sr=87,6	Ba=137	Pb=207.
		?=45	Ce=92		
		?Er=56	La=94		
		?Yt=60	Di=95		
		?In=75,6	Th=118?		

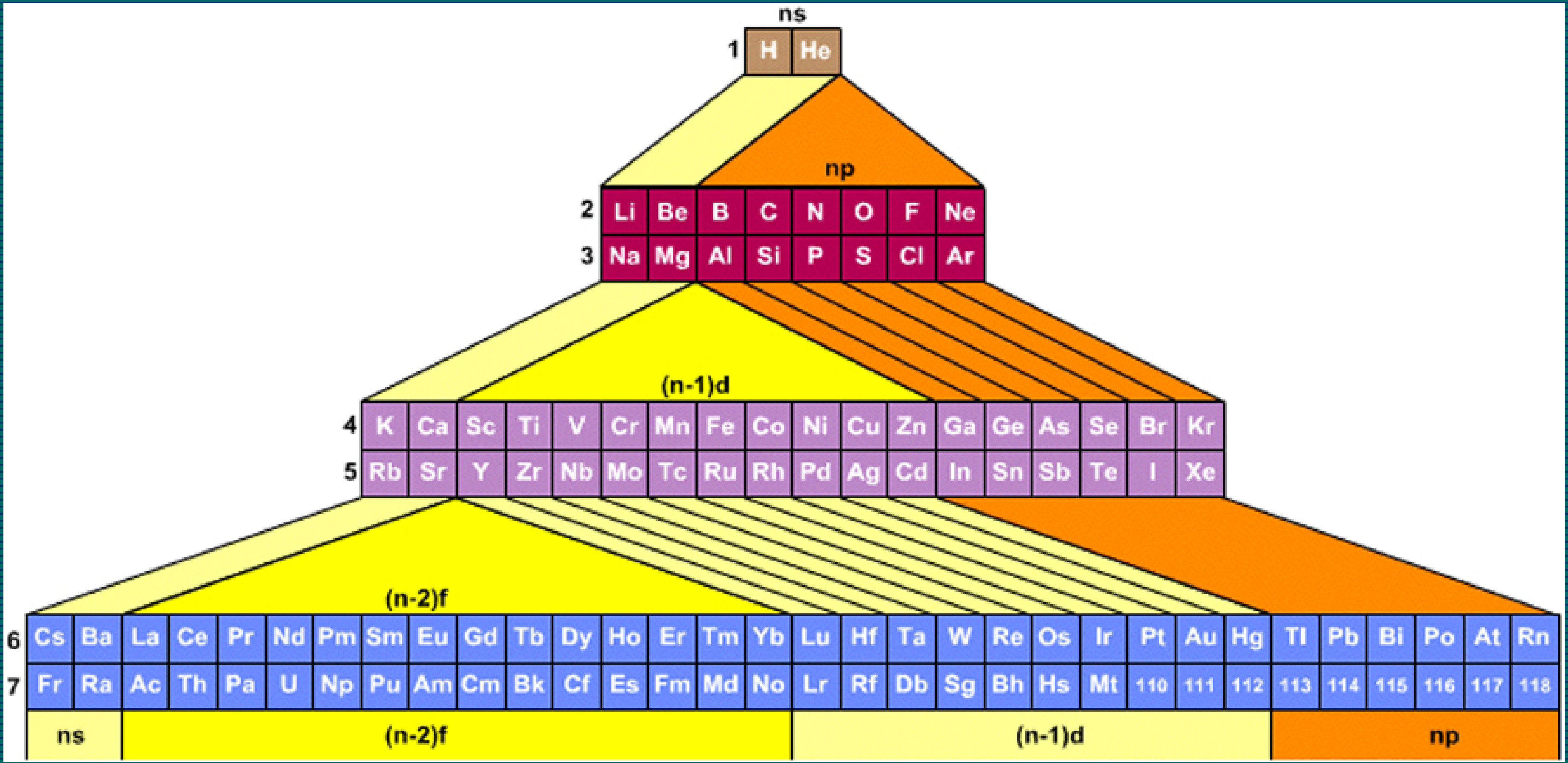
Dimitri Mendeleev’s periodic table of 1869



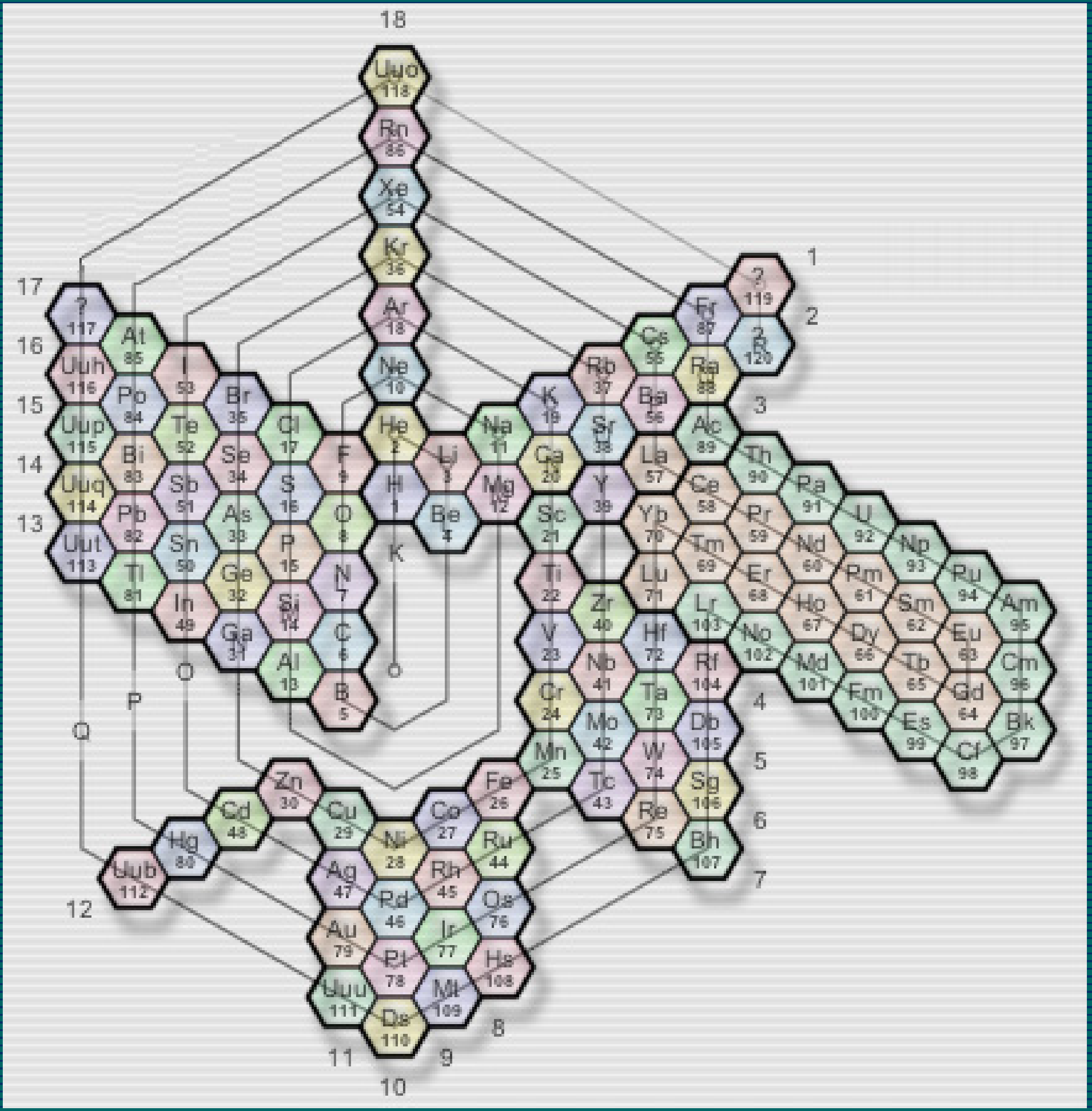
Charles Janet’s periodic table of 1927



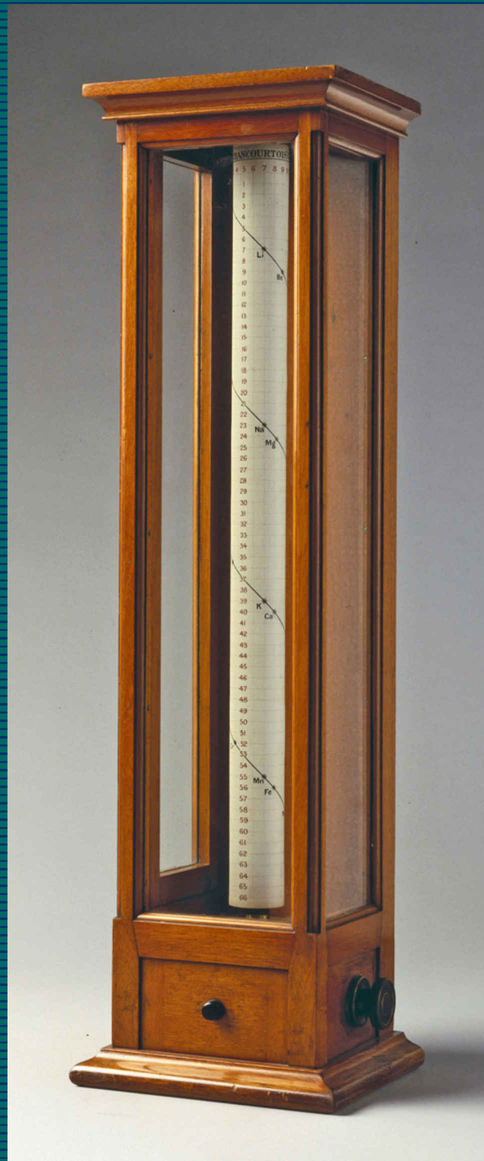
Contemporary Periodic Table by U.S. NIST

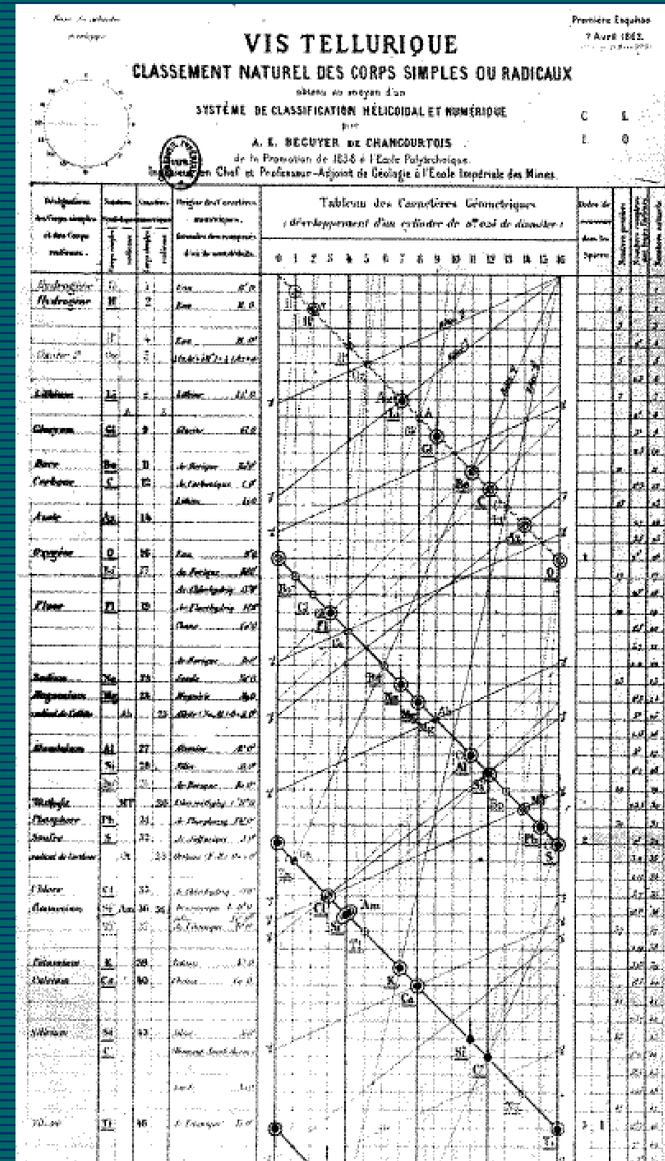


Bayley-Thomsen-Bohr Periodic Table of 1882, 1895, 1922, & 1989

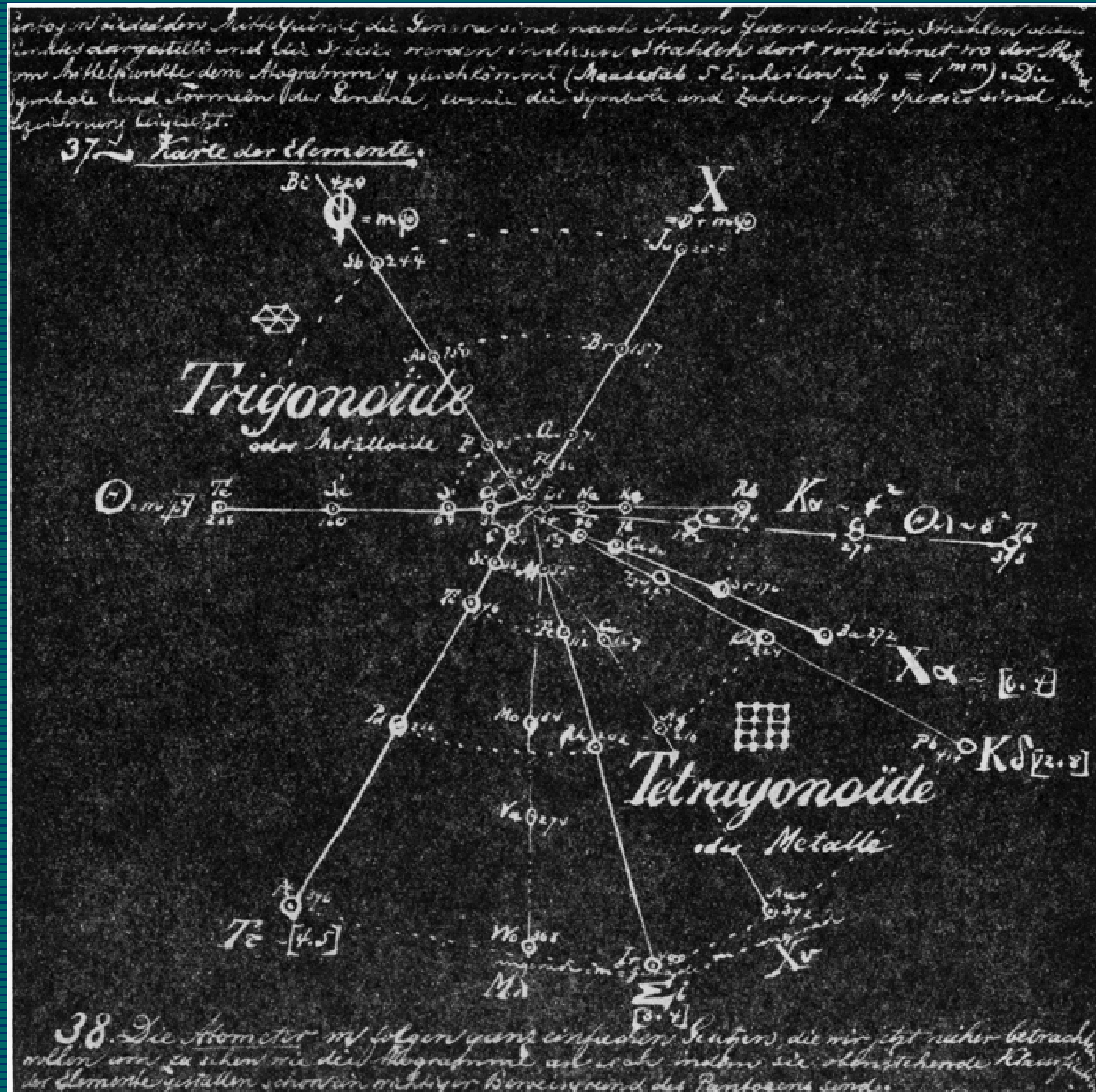


Periodic Spiral by Electric Prism, Inc.

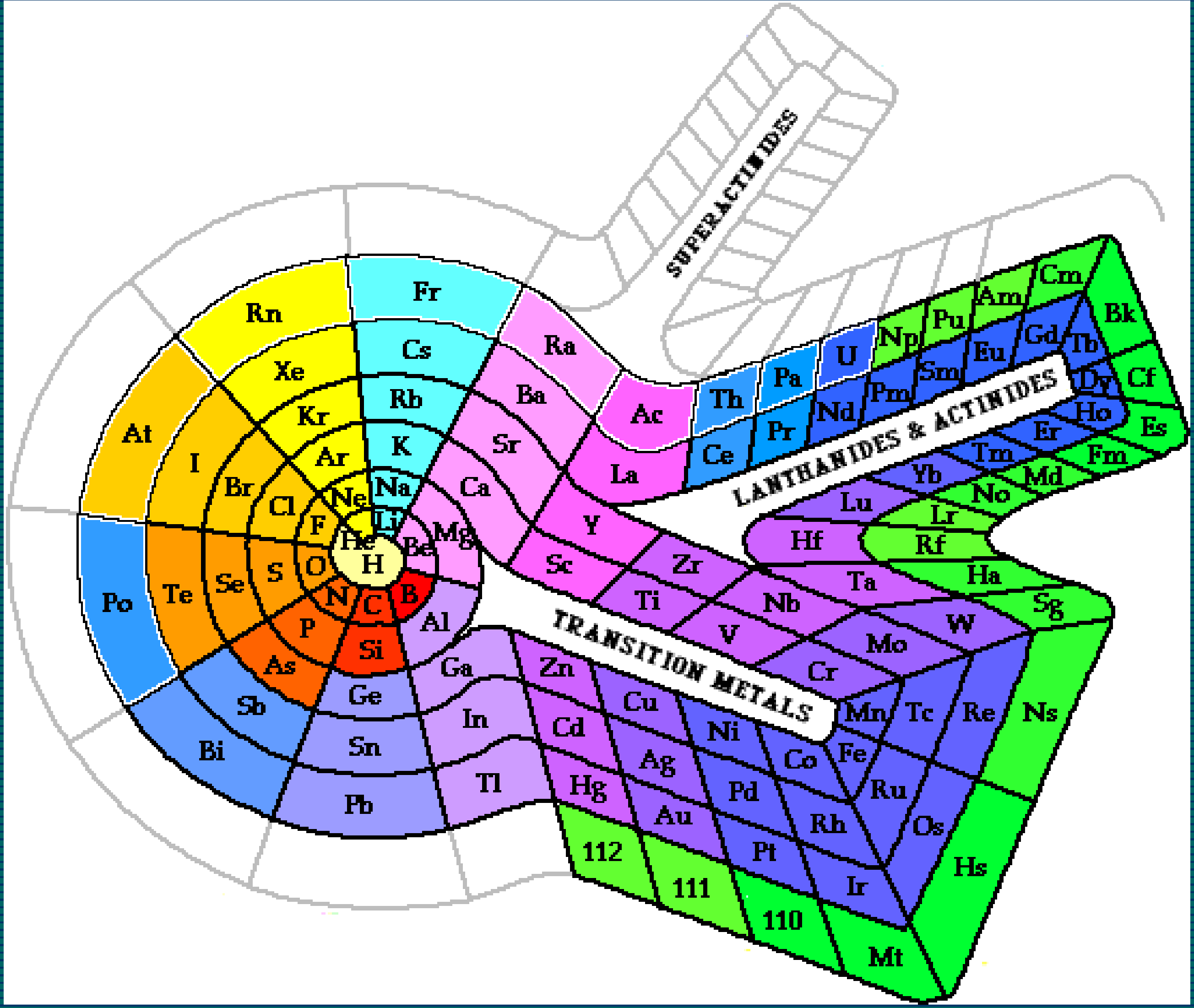




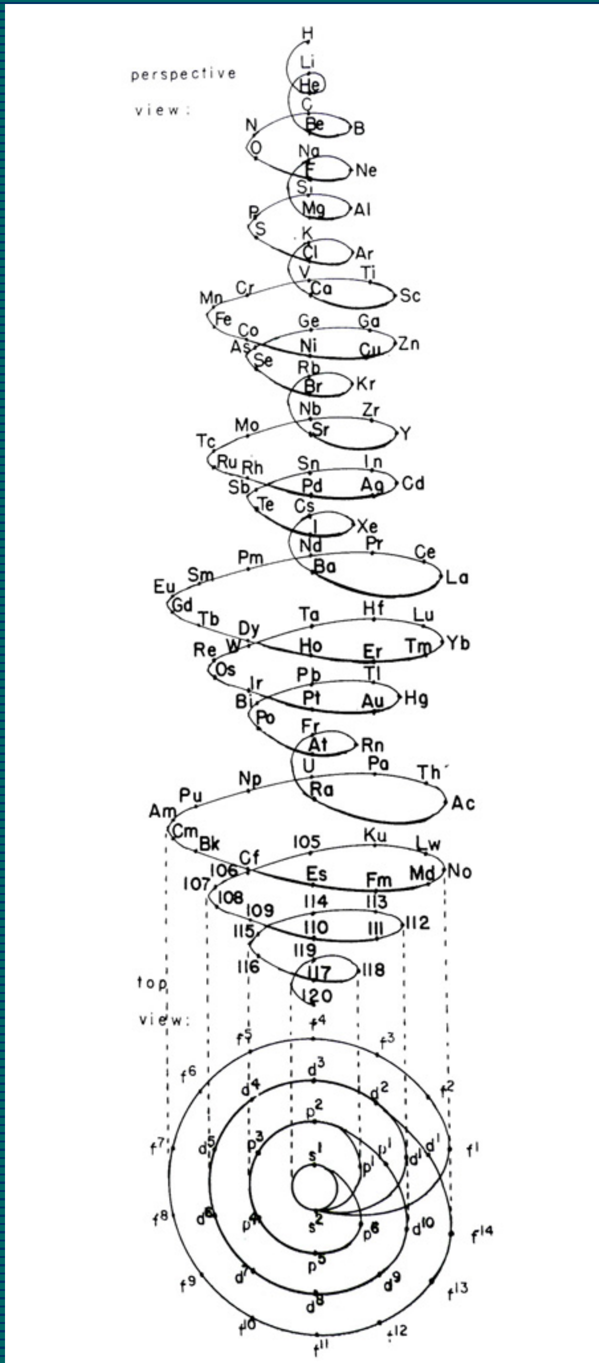
Alexandre-Émile Béguyer de Chancourtois's Telluric Screw, 1862.



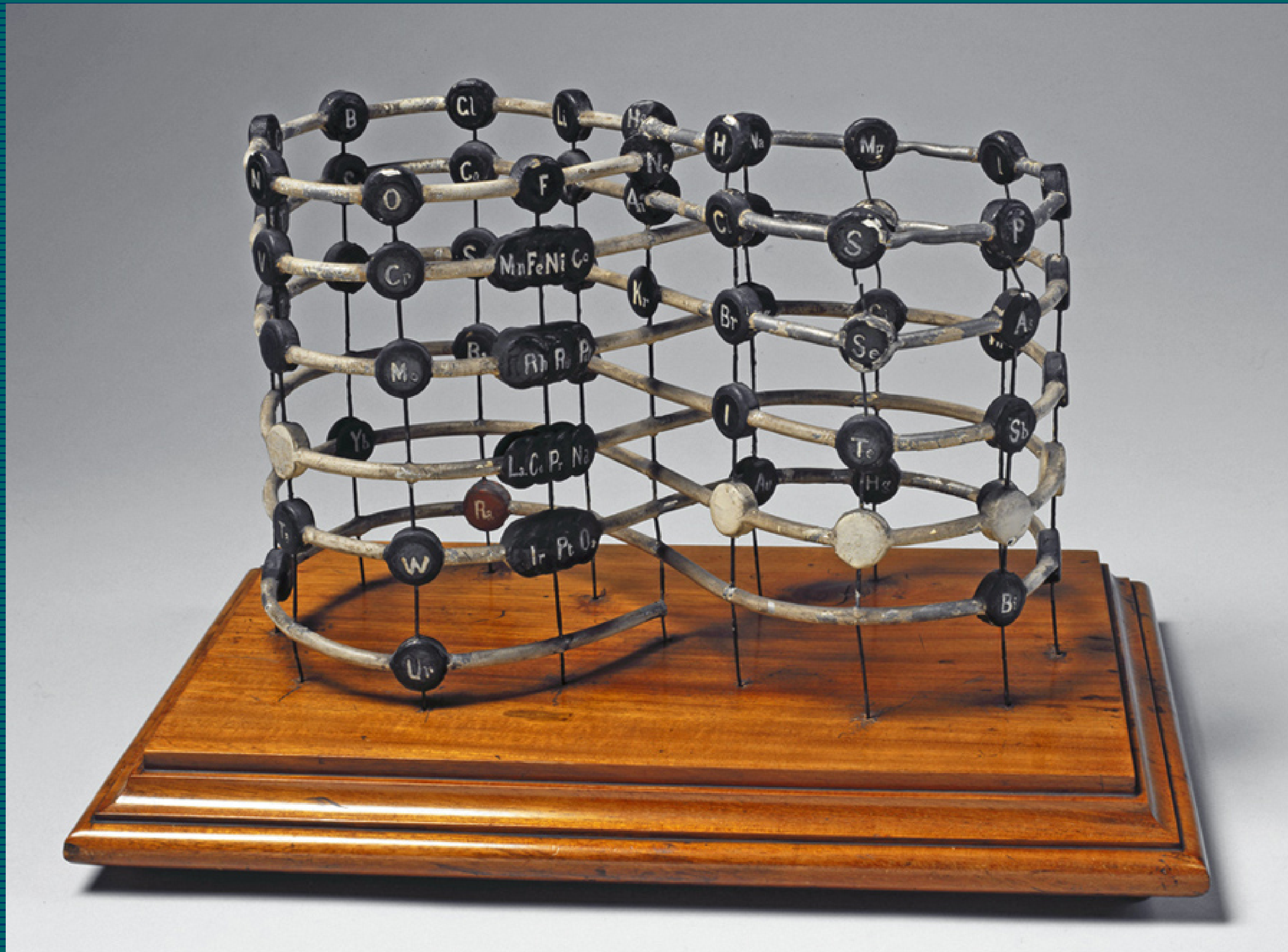
Gustavus Detlef Hinrichs’s spiral/radial alignment, 1867



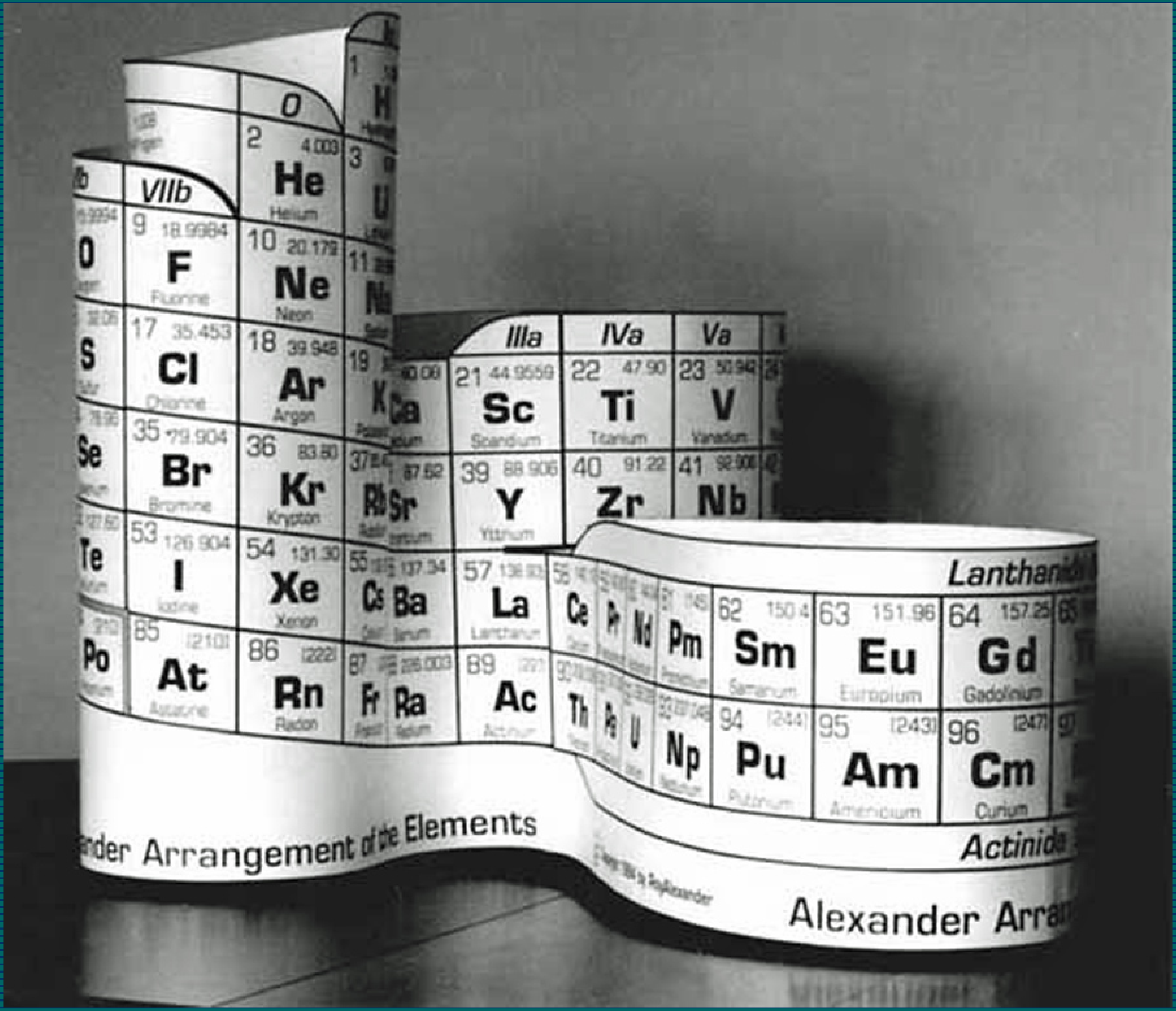
Theodor Benfey’s spiral table of 1960.



Georg Schaltenbrand’s helices of 1920



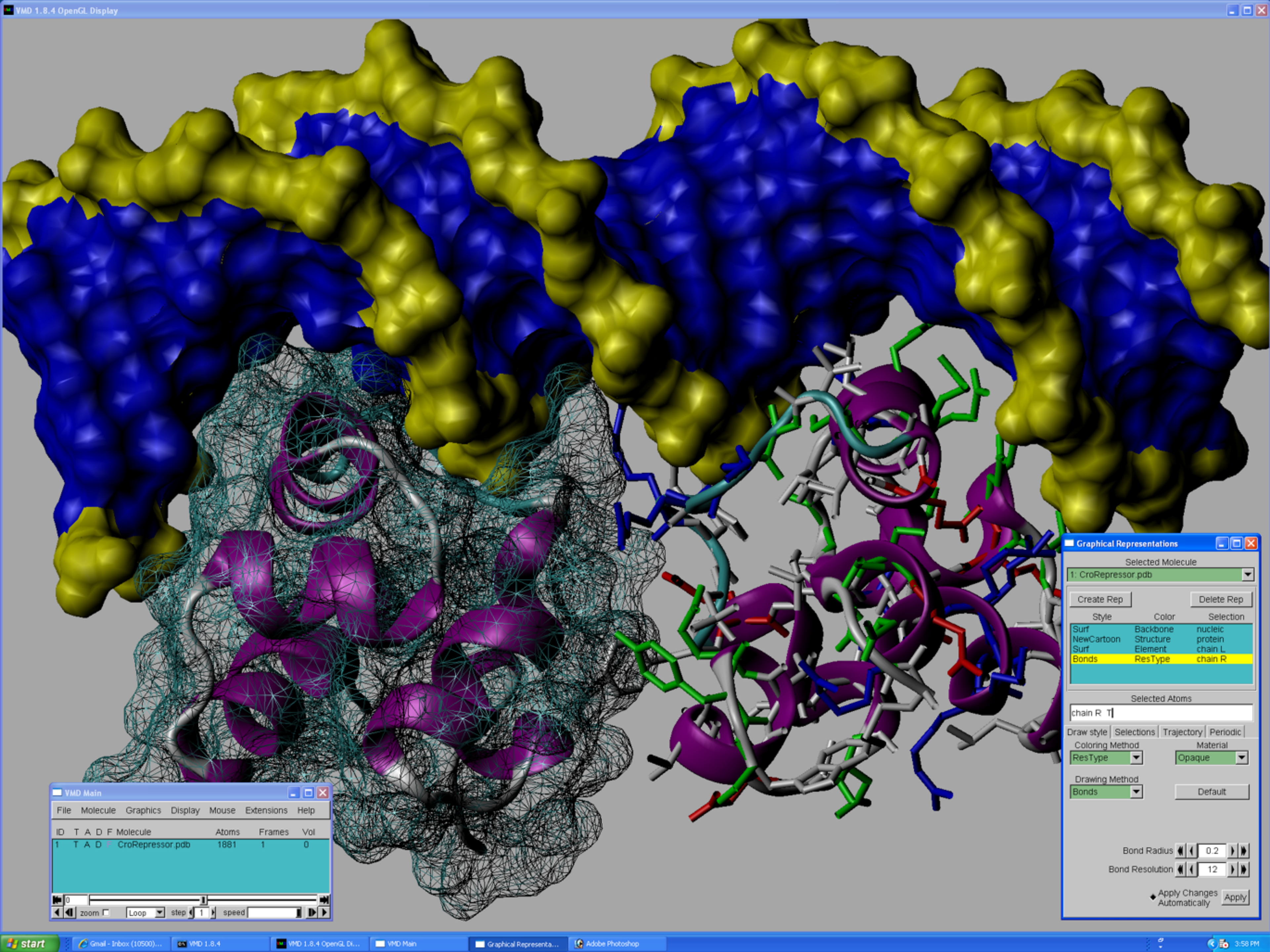
William Crooke’s *pretzel* model of 1888.



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


VMD 1.8.4 OpenGL Display
Graphical Representations
Selected Molecule
1: CroRepressor.pdb
Create Rep
Delete Rep
Style
Color
Selection
Surf
Backbone
nucleic
NewCartoon
Structure
protein
Surf
Element
chain L
Bonds
ResType
chain R
Selected Atoms
chain R T
Draw style
Selections
Trajectory
Periodic
Coloring Method
Material
ResType
Opaque
Drawing Method
Bonds
Default
Bond Radius
0.2
Bond Resolution
12
Apply Changes Automatically
Apply
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID
T
A
D
F
Molecule
Atoms
Frames
Vol
1
T
A
D
CroRepressor.pdb
1881
1
0
zoom
Loop
step
1
speed
start
Gmail - Inbox (10500)...
VMD 1.8.4
VMD 1.8.4 OpenGL Di...
VMD Main
Graphical Representa...
Adobe Photoshop
3:58 PM

Electronegativities

Explore the **electronegativity** of the chemical elements through this periodic table

Group / Period	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

*Lanthanoids	*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
**Actinoids	**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

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

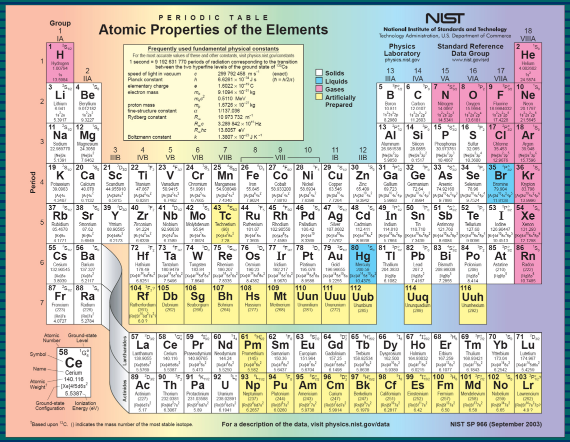
- Must reflect kinds of questions asked of the data it contains.
- Three levels of inquiry:
  1. Elementary questions about data:
     - single category data inspection or extraction
  2. Intermediate questions about data:
     - comparisons, trends, and relationships among data entries
  3. General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

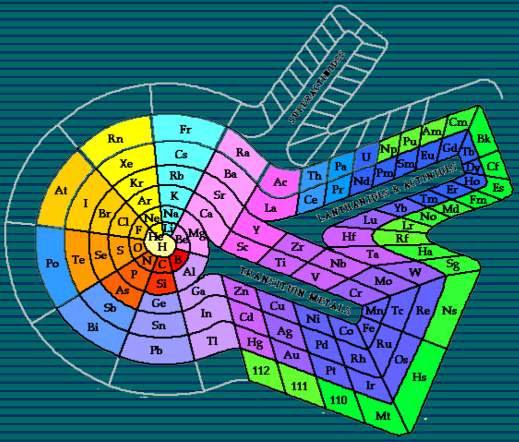
Analysis of Modern *Table Design*

- 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



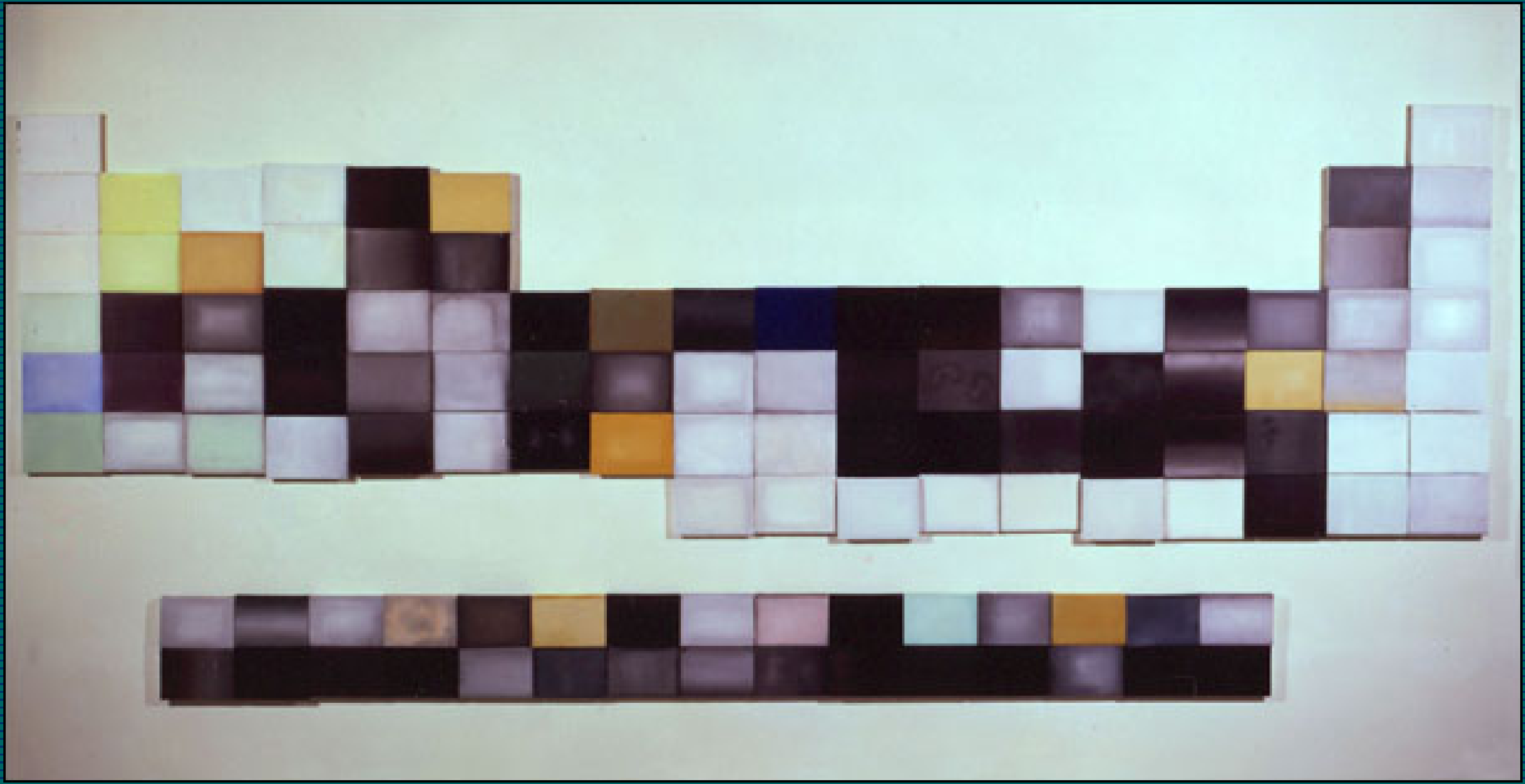


Further requirements for Hypermedia Tables

- 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 two-dimensional 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 !