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News from the Periodic Table: An Introduction to “Periodicity Symbols, Tables, and Models for Higher-Order Valency and Donor–Acceptor Kinships”

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This article is an abbreviated overview of the full article that is available in Supplemental Material.^W The overview briefly outlines the formal physico–mathematical basis of chemical *Aufbau* and summarizes modern quantum chemical evidence for “higher-order” periodicity patterns that emphasize the deep *commonality* of chemical versus spectroscopic characterizations, often perceived as adversarial. We highlight limitations of the current IUPAC-approved periodic table and suggest a variety of alternative tabular and non-tabular forms that is hoped to elicit ongoing discussions at the companion *JCE Forum* for this article. We also suggest pedagogical exercises that encourage creative exploration of the richness of atomic valency and bonding patterns, even at an elementary level. Throughout this introductory overview, the literature citations, equations, and figure numbers pertain to the full-length article available in Supplemental Material.^W

Evolving Table: Quantum Links

Chemistry is a quantum mechanical phenomenon. Advances in quantum chemical technology may therefore be expected to continually enrich our understanding and teaching of chemical phenomena. The deep relationship between quan-

tal electronic *Aufbau* principles and atomic valency and bonding regularities is most familiarly expressed in the Mendeleev-style periodic table, the signature icon of chemistry classrooms. However, certain aspects of the standard (IUPAC-approved) periodic table appear suboptimal for representing the underlying electronic logic of chemical periodicity as currently understood. In this respect, spectroscopic-type tables with closer links to the underlying quantum numbers, such as Janet’s left-step table (Figure 1^W) and others discussed below, appear to have significant advantages.

What features of electronic valency and bonding should a graphical depiction of chemical periodicity aim to display, and how are the corresponding trend-lines exhibited in various tabular layouts? Of primary importance are the deep associations with the n and l quantum numbers of the atomic valence shell orbitals and the familiar Madelung ($n + l$) rule for their energetic ordering. The theoretical basis for the Madelung *Aufbau* sequence is derived (eqs 1–4^W) from the general Sturm–Liouville theory of single-configuration wave equations. This theory allows one to uniquely associate the energy ordering with the number of radial and angular *nodes* in each valence orbital. Such *Aufbau* node-counting involves both the number and strength (indicial multiplicity) of radial

																		H 1	He 2												
																		Li 3	Be 4												
																		B 5	C 6	N 7	O 8	F 9	Ne 10	Na 11	Mg 12						
																		Al 13	Si 14	P 15	S 16	Cl 17	Ar 18	K 19	Ca 20						
														Sc 21	Ti 22	V 23	Cr 24	Mn 25	Fe 26	Co 27	Ni 28	Cu 29	Zn 30	Ga 31	Ge 32	As 33	Se 34	Br 35	Kr 36	Rb 37	Sr 38
														Y 39	Zr 40	Nb 41	Mo 42	Tc 43	Ru 44	Rh 45	Pd 46	Ag 47	Cd 48	In 49	Sn 50	Sb 51	Te 52	I 53	Xe 54	Cs 55	Ba 56
La 57	Ce 58	Pr 59	Nd 60	Pm 61	Sm 62	Eu 63	Gd 64	Tb 65	Dy 66	Ho 67	Er 68	Tm 69	Yb 70	Lu 71	Hf 72	Ta 73	W 74	Re 75	Os 76	Ir 77	Pt 78	Au 79	Hg 80	Tl 81	Pb 82	Bi 83	Po 84	At 85	Rn 86	Fr 87	Ra 88
Ac 89	Th 90	Pa 91	U 92	Np 93	Pu 94	Am 95	Cm 96	Bk 97	Cf 98	Es 99	Fm 100	Md 101	No 102	Lr 103	Rf 104	Db 105	Sg 106	Bh 107	Hs 108	Mt 109	Ds 110	Rg 111									

f

d

p

s

Figure 1. Left-step table of the chemical elements, showing horizontal Madelung tiers (l) and vertical l -block group (le) assignments.

or angular sign-crossings, which are conveniently depicted in a mnemonic *atomic valence node*, AVN, symbol for each element (Figures 2 and 3^W). The angular pie-slices, radial concentric circles, and electronic dots of the AVN symbol uniquely identify the position of the element in the Madelung sequence according to angular *l* blocks (s, p, d, and f groups) and radial “tier” of its occupied valence orbitals. The characteristic misalignment of He with p-block elements is a conspicuous defect of the conventional IUPAC-style depiction of AVN patterns.

Higher-Order Patterns

Five additional “higher-order” periodicity patterns are described that are also unnecessarily obscured in the IUPAC-style tabulation:

- (1) The occupied (donor) and unoccupied (acceptor) valence orbitals of each element allow one to recognize iso-donor and iso-acceptor kinships between elements of different *l* blocks (ref 13^W). These can be effectively represented by a step-pyramid table (Figure 4^W) or related graphical devices (Figures 11–13^W) to indicate valency parallels between *l* blocks.
- (2) The recent discovery (refs 5 and 14^W) of profound Lewis-like analogies between p-block and d-block compounds allows one to identify hypovalent versus normal-valent counterparts of each angular subblock, as well as direct iso-valency relationships between *l* blocks (connecting, e.g., C with Os). Such Lewis-like kinships call attention to the unique role of the s block in hybridized bonding, as displayed, for example, in the 3D “periodic towers” model described below.
- (3) The direct association of increased metallicity, that is, decreased effectiveness of directional hybridized bonding, with increased radial and angular nodal character leads to a conspicuous metallicity trend from upper right to lower left in each angular subblock of nonzero *l* (the s block being uniquely excluded from such hybridization trends, as noted above). The corresponding trend-lines for electronegativity, that is, the competition for electrons in directional hybridized bonding, are also rendered consistently within each *l* block (Figure 5^W), provided that H, He are restored to proper AVN s-block positions.
- (4) Vertical Dobereiner-type triad relationships (of the type first recognized about a half-century before Mendeleev’s earliest periodic table) and the associated nobility trends for terminal closed-shell atoms of each *l* block allow surprisingly accurate “atom-analogy” interpolations (eqs 9 and 10^W) within chemical families, provided again that H, He occupy properly aligned AVN positions. Practical exercises in using such triad relationships serve to illustrate many interesting aspects of chemical interpolation or extrapolation to unknown property values and elements.
- (5) The important “rule of first-element distinctiveness” (refs 13 and 19^W) can be traced to the profound effects of inner-core steric or orthogonality repulsions for all but the

first member of each *l* block. The associated trend-line of distinctiveness with respect to vertical congeners,

s block >>> p block >> d block > f block

is exhibited conspicuously (Figures 5–8^W) in the left-step and other AVN-aligned tables, but scrambled in the conventional IUPAC-style table.

Discussion

From these examples, we can recognize that the current IUPAC-style layout obscures both primary and higher-order patterns of considerable chemical significance, particularly by misplacing He with the p block. The professed reasons for grouping He with p-block terminal elements, based on superficial similarities of gaseous phases at standard-state conditions, can be recognized as violating Mendeleev’s expressed goal of displaying the intrinsic reactive propensities of *atoms* rather than the physical resemblances of pure elemental *substances*. Subsequent theoretical recognition of the intimate relationship between chemical reactivity and optical or ionization spectroscopy has largely obviated earlier justifications for distinguishing “chemical-type” versus “spectroscopic-type” tables of atomic periodicity.

Finally, our article suggests some alternative 2D, 3D tables or models that seem to better represent the higher-order periodicity patterns in AVN-consistent manner. These include a 3D AVN-space model (Figure 9^W), a helix-on-cylinder model (Figure 10^W), and the articulated periodic-towers model (Figure 11–13^W). The latter seeks to emphasize the Lewis-like bonding analogies between *l* blocks (refs 5 and 14^W) through “side-wing” (hypovalent) versus “tower” (normal-valent) structural features of the 3D winding pattern. Indeed, armed with no more than a ribbon of sequential elemental AVN symbols and a scissors, elementary students are often able to snip and arrange the ribbon segments into AVN-consistent blocks that better exhibit the higher-order periodicity trends than does the standard IUPAC-style table! Additional exercises and studies related to chemical periodicity are described in a recent monograph by one of the authors (1). In the spirit encouraged by Mendeleev, we believe that alternative tabular or model forms can bring “fresh energy” to effective depiction of chemical periodicity patterns, while also improving their pedagogical consistency with underlying wave-mechanical principles that govern electronic behavior.

^WSupplemental Materials

The full-length article is available in this issue of *JCE Online*. A companion “Periodic Table” *JCE Discussion Forum*, co-hosted by Henry Bent and Frank Weinhold, is found at <http://forums.jce.divched.org:8000/JCE/>.

Literature Cited

1. Bent, H. *New Ideas in Chemistry from Fresh Energy for the Periodic Law: An Introduction to Leading Uses of the Left-Step Periodic Table*; Authorhouse: Bloomington, IN, 2006.