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A QUANTUM MECHANICS CONSISTENT PERIODIC TABLE

ABSTRACT

Almost all periodic tables of the chemical elements are between 96 % and 100 % in accord with quantum mechanics. Three elements only do not fit correctly into the official tables, in disagreement with the Pauli exclusion principle. In order to ensure coherence, it is put forward to place helium beside hydrogen into the s-block instead of the p-block. Lutetium and lawrencium pertain to the d-block of the transition metals and should not be in the f-block with the rare earths or the actinoids. With these slight modifications, the IUPAC table becomes entirely quantum mechanics consistent. This does not mean that the periodic table is entirely explained by quantum mechanics, based on ad hoc principles. Plausible explanations of those have been attempted.

KEYWORDS

Periodic table - Spherical harmonics - Madelung rule - Helium - Lutetium - Lawrencium

INTRODUCTION

The purpose of this paper is to find the necessary characteristics of a quantum mechanics consistent periodic table, neglecting electron spin, "except that we adopt the exclusion principle" (see Feynman, 1966, p. 19.14). There are a great variety of periodic tables due to the various graphical, mathematical, physical or chemical criterions used. We shall compare some tables with respect to quantum mechanics and produce one, slightly modified from the official International Union of Pure and Applied Chemistry (IUPAC) table, by applying the Schrödinger theory of the hydrogen atom combined with the Bohr Aufbau principle (lowest energy), Pauli exclusion principle (pairing), Hund's rule (equal energy) and Madelung rule ($n + \ell$).

SHORT HISTORY OF THE PERIODIC TABLE

The Mendeleev table is more than one century old. It was originally based on atomic masses with twelve lines and eight columns, corresponding already but partially to the blocks s (groups I and II), p (groups III, IV, V, VI and VII) and d (III, IV, V, VI, VII, VIII) of quantum mechanics. The transition metals were moved separately and the rare gases replaced the corresponding column after their discovery by Ramsay. Moseley replaced the mass with the atomic number as a classification criterion. The transuranians were discovered by Seaborg who placed the lanthanoids and actinoids separately, below the table, for reasons of compactness. In 1985 the IUPAC Commission on the Nomenclature of Inorganic Chemistry proposed a new notation for the groups of the periodic table where the numbering of the groups was changed from VIII groups to 18 columns. "The new group numbers are the sum of s + p + d electrons after the last noble gas" (Fluck, 1988). f is missing: the present IUPAC periodic table is therefore not quantum mechanics consistent.

CHARACTERISTICS OF A QUANTUM CONSISTENT TABLE

Each element is represented in the correct block (s, p, d or f). Helium is in the p-block. The lanthanides and actinides may be in a separate group of columns corresponding to the f-block, recalled in an independent column. In each row appears only one atomic shell (K, L, M, N, O, P or Q) e.g. with the same principal quantum number n (1, 2, 3, 4, 5, 6 or 7). This seems to be possible only for the first three rows with continuous increase of the atomic numbers from left to right. In the next four rows the d-subshells are one row too low and the f-subshells are two rows too low in the table. The elements in even and uneven columns are paired according to the Pauli exclusion principle; therefore, each block contains an even number of elements. The detailed electronic structure may show local anomalies without impact on the structure of the periodic table.

VARIOUS TABLES

Although updated many times, many periodic tables still have some inconsistencies shown in grey on table 1. There is a vacant box beside hydrogen and a strange discontinuity below yttrium. The columns of the lanthanides and actinides are not numbered.

| ℓ | s-block | | d-block | | | | | | | | | | p-block | | | | | |
|--|---------|-------|---------|-------|-------|-------|-------|--------|-------|-------|-------|----------|---------|-------|-------|-------|-------|-------|
| | 0 | | 2 | | | | | | | | | | 1 | | | | | |
| Number of electrons (except anomalies) $1, 2 \dots 2(2\ell + 1)$ | 1 | 2 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 | 2 | 3 | 4 | 5 | 6 |
| Spectroscopic | s^1 | s^2 | d^1 | d^2 | d^3 | d^4 | d^5 | d^6 | d^7 | d^8 | d^9 | d^{10} | p^1 | p^2 | p^3 | p^4 | p^5 | p^6 |
| Los Alamos | 1A | 2A | 3B | 4B | 5B | 6B | 7B | 8B | | 11B | | 12B | 3A | 4A | 5A | 6A | 7A | 8A |
| CAS or US | IA | IIA | IIIB | IVB | VB | VIB | VII B | VIII B | | IB | | IIB | IIIA | IVA | VA | VIA | VIIA | VIIIA |
| Ancient IUPAC or European | IA | IIA | IIIA | IVA | VA | VIA | VIIA | VIIIA | | IB | | IIB | IIIB | IVB | VB | VIB | VII B | VIIIB |
| IUPAC groups | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| Periods and shells | | | | | | | | | | | | | | | | | | |
| 1 \square K | H | | | | | | | | | | | | He | | | | | |
| 2 \square L | Li | Be | | | | | | | | | | | B | C | N | O | F | Ne |
| 3 \square M | Na | Mg | | | | | | | | | | | Al | Si | P | S | Cl | Ar |
| 4 | K | Ca | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | As | Se | Br | Kr |
| 5 | Rb | Sr | Y | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | I | Xe |
| 6 | Cs | Ba | La...Lu | Hf | Ta | W | Re | Os | Ir | Pt | Au | Hg | Tl | Pb | Bi | Po | At | Rn |
| 7 | Fr | Ra | Ac...Lr | Rf | Db | Sg | Bh | Hs | Mt | Ds | Uuu | Uub | 113 | Uuq | 115 | Uuh | 117 | Uuo |

| $2(2m + 1)$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|-------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 6 | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu |
| 7 | Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | Lr |

Table 1. On the IUPAC official table, there are 7 rows or periods and 18 columns or groups (see Holden, 2004; Cohen, 2007; Leigh, 2001). Anomalies with respect to quantum mechanics are shown in gray. Various methods of numbering the columns are shown. Columns 3 to 12 form the d-block, the transition metals, formerly part of Mendeleev group VIII. Column VIIIA or VIIIB used for the rare gases was renamed 18. The f-block is apart and seems to have no column numbering. At the top appears the numbering based on the azimuthal quantum number ℓ (also called second quantum number or orbital angular momentum quantum number). In the spectroscopists' notation, the azimuthal quantum number ℓ is replaced by a letter (s, p, d or f) used to name the blocks. The magnetic quantum number m or m_l corresponds to the possible properties of an electron in a magnetic field. "The superscript (...) represents the multiplicity of the energy levels" (Pauling, 1989, p. 42).

The first three rows coincide with the first three atomic shells: K, L or M. The next four periods have mixed hydrogen shells. Therefore, the hydrogen model works fine for the first three periods only.

The positions of H, He, La and Lr vary, depending on the taste of the authors of the tables (table 2). A strong minority of tables have Lu and Lr in the d-block (columns 3 to 12) and He in the s-block (column 2). Some say that He is in the s-block, but put it at the right, in column 18, corresponding to the p-block. Bent recommends to place He above Be without clear reference to quantum mechanics (Bent, 2006, p. 80). Hydrogen is sometimes placed in the middle of the table, saying that it could be as well in group 1 or 17 (Jensen, 1982; Atkins, 2002, endpaper). Some place hydrogen in both groups 1 and 17 (Kotz, 1991, endpaper and p. 342). Lanthanides and actinides are diversely connected to the main table, either to column 3 or to one of its edges.

Table 2: Quantum consistency of periodic tables found in the literature

| s-Block | p-Block | d-Block | f-Block | Table type | Remarks | % QM consistent | Reference |
|---------|---------|---------|-------------------|------------------------------|-------------------------|-----------------|--|
| H, He | | Lu, Lr | | Left-step or pyramidal | s-Block at the right | 86 % or 100 % ? | Janet, 1930; see Scerri, 2007 p. 283, 284; Scerri, 2005; Bent, 2006, p. 69 |
| | H, He | | Lu, Lr | Medium long form | Post-Seaborg | 96 % | see Scerri, 2007 p. 23 |
| H | He | | Lu, Lr | Medium long form | La, Ac duplicated | 97 % | Wichman, 1971, p. 121 |
| H | He | | Lu, Lr | Medium long form | IUPAC | 97 % | Cohen, 2007, endpaper |
| | H, He | Lu | | Short period system | Table ends at Z = 101 | 98 % | Born, 1989, p. 39 |
| | H, He | Lu, Lr | | Medium long form | | 98 % | Watson, 2008, p. 2 |
| | He | Lu, Lr | | Medium long form | H in the middle | 98 % | Jensen, 1982 |
| He | | Lu, Lr | | Medium long form | H in the middle | 99 % | Atkins, 2002, endpaper; see Scerri, 2005 |
| H, He | He | | Lu, Lr | Special | | 99 % | Pauling, 1988, p. 135 |
| H | He | Lu, Lr | | Medium long form | Popular table | 99 % | McQuarrie, 1992, p. 336; see Scerri, 2007 p. 13; 1998b |
| H | | Lu, Lr | | Long form | With triads | 99 % | see Scerri, 2007 p. 181 |
| H, He | | Lu, Lr | | Spiral, pyramidal, long form | With subshells | 100 % | Ouahès, 1995, p. 109, 119, endpaper |
| H, He | | Lu, Lr | | Medium long form | H duplicated in p-block | 100 % | Kotz, 1991, endpaper |
| H, He | | | | Vertical | Table ends at Z = 36 | 100 % | Feynman, 1966, p. 19.15 |
| H, He | | Lu | | Vertical & pyramidal | Lr unknown | 100 % | Bohr, 1923b, p. 10, 34 |

Table 2. The problem of the periodic tables lays essentially on the position of the three elements He, Lu and Lr. Here, the various periodic tables have a 1 % error for each element in the wrong block (according to the quantum mechanics of the hydrogen atom). All periodic tables are almost quantum mechanics consistent; they only need a few corrections. Almost all possible combinations of H, He, Lu, Lr are found in this table. Some authors tell correctly to which block pertains an element but put it incorrectly in the table or, when in doubt, at two different places or show different versions of the periodic table.

The Janet or left step table seems, at first glance, to be quantum consistent but none of its s-block and p-block elements are in the same atomic shell (Janet, 1930; see Scerri, 2007, p. 283). Anyway, the rows and shells, in rows 4 to 7, will never coincide because the structure of the hydrogen atom is only adequate for the first three shells, K, L, M. The pyramidal table (Bohr, 1923b) is usually correct but not very practical. The modified version is equivalent to the Janet table with the s-block on the right-hand side (see Scerri, 2007, p. 284).

Vertical tables, with the electronic configuration of the atoms, usually called periodic system, have the elements listed vertically with one element per line, in the order of their atomic numbers (see Feynman 1966, p. 19.15; Wohl, 2005; Born, 1989, p. 181). For that reason, they are automatically quantum mechanics consistent. They show the anomalies of the electronic structure, useful to predict the physical and chemical properties of the elements but without influence on the structure of the periodic table. In order to have 100 % quantum mechanics consistent periodic tables, all the elements must be shown in the correct block,

(s, p, d, or f corresponding to the azimuthal quantum number ℓ). This is not the case for the official IUPAC table where helium appears in column 18 corresponding to the p-block instead of column 2 in the s-block; lutetium and lawrencium appear in the separated f-block and not in the d-block, column 3.

PERIODIC TABLE AND ELECTRONIC STRUCTURE

The complete electronic structure of the atom is necessary to predict the physical and chemical properties of the elements. Some elements have configuration anomalies in the electronic sequence. For example chromium has the following electronic structure $[\text{Ar}] 4s^1 3d^5$ and not the expected one, $[\text{Ar}] 4s^2 3d^4$. This does not change the structure of the table because copper and chromium are in the middle of the d-block. Helium, lutetium and lawrencium, being at the boundary of their blocks, it is important to analyze their position.

Helium

It is well known that helium has a $1s^2$ structure, a spherical mode of vibration, the same as hydrogen $1s^1$; the difference is in the number of electrons two instead of one (see Wichmann, 1971, p. 122). Helium, pertaining to the s-block of the K-shell, is usually placed with the other rare gases at the right of the table where the electronic structure of the outermost subshell is np^6 with six electrons instead of two for helium. "Helium has just two outer electrons and might therefore be placed among the alkaline earth metals such as magnesium and calcium" (see Scerri, 2005, p. 136). Moreover, as Bartlett has shown, the noble gases are not so inert. There exist compounds of xenon and krypton with fluorine, chlorine, hydrogen, platinum (Bartlett, 1962), gold (Brisdon, 2001) ... There is no chemical reason any more to place helium with the other noble gases. Some authors put He in the p-block by writing the electronic structure as $1s^2 p^0$. p^0 has no meaning: it contains no electron; the electronic structure of He is $1s^2$ and that's all. There is a vacant box beside hydrogen waiting for helium where it has its natural place.

Helium may be called a s-block noble gas, defined by its filled outer subshell of valence electrons in the s-block but cannot appear in the p-block e.g. in column 18.

Lutetium and lawrencium

Lutetium and lawrencium are traditionally considered as belonging respectively to lanthanoids and actinoids having 15 elements each (see Wichmann, 1971, p 121; Fano, 1959, p. 172). Born considers lutetium as a transition metal although he recognizes that there is an alternative possibility suggested by Seaborg (see Born, 1989, p. 183; Scerri, 2007 p. 23).

The d-block contains 10 elements, not 24 as it looks like on the IUPAC table where there is no distinction between the d and f blocks. Ytterbium (Xe) $4f^{14} 6s^2$, with all its shells closed, is the end of the 4f subshell of the lanthanides with 14 electrons. Lutetium has the structure (Xe) $4f^{14} 5d^1 s^2$, already found by Bohr and Coster (Bohr, 1923a). It has the first electron of the 5d subshell of the transition metals (Bohr 1923b). The same thing happens for lawrencium. Now the Pauli exclusion principle is fulfilled: the f-block, without Lu, contains an even maximum of 14 electrons and the four rows of the d-block have 10 elements. Lutetium (named Casseopeium Cp by Bohr) pertains thus to the d block of the transition metals with 10 elements and therefore not to the f-block of the lanthanoids. This is also valid for the actinoids, mostly unknown at the time of Bohr. A physical or chemical classification criterion seems difficult to apply to the newly discovered actinoids that decay seconds after they are formed (Kendall, 2002). Strange et al. did not include lutetium in their study of the valence of rare earths (Strange, 1999). "All of these properties unanimously favor the placement of lutetium and lawrencium, rather than lanthanum and actinium, in group VIII B" (Jensen, 1982).

Lutetium and lawrencium may be called lanthanoid and actinoid of the d-block but cannot appear within the f-block with the other rare earths.

BOHR THEORY (1913)

The Bohr theory of the hydrogen atom describes accurately the energy levels of the hydrogen atom and the Balmer series with circular trajectories of the electrons (Bohr 1923b, p. 15). The electrons move around the nucleus like planets around the sun with a supplementary condition: the angular momentum should be equal to $n \hbar$, where \hbar is Planck's constant divided by 2π and n an integer. The solutions of the Bohr theory are circles and the energies E_n are given by:

$$\frac{1}{2}m_e v_n^2 = E_n - \frac{1}{4\pi\epsilon_0 r_n} = E_n - \frac{R_H}{n^2} = \frac{R_H}{2n^2}$$

where R_H is the Rydberg constant, m_e is the mass of the electron, v_n its velocity r_n its radial position and ϵ_0 the permittivity of the vacuum. Sommerfeld generalized it to elliptical trajectories and applied a relativistic correction.

WAVE MECHANICS THEORY OF THE HYDROGEN ATOM (1926)

Schrödinger developed a wave equation whose solutions are standing waves similar to the standing waves in a spherical resonator (Schrödinger, 1926). Born compares the hydrogen atom with a "circular membrane fixed at the circumference. The number of radial nodal lines (...) is the quantum numbers of the state of vibration" (Born 1989, p. 139). The hydrogen nucleus with its electrostatic potential may be compared to a pond limited by a slope. The waves propagate at a variable velocity, like that of a tsunami function only of the water depth. The velocity of the matter waves (de Broglie, 1925) depends only on the velocity of the electron which depends on its initial velocity and on the electrostatic potential, like a comet being captured by the sun if its velocity is smaller than the escape velocity. An electron approaching a proton will be captured in the same conditions, the difference is that it has to lose some energy by radiation until its angular momentum be exactly $n\hbar$. In the Schrödinger theory of the hydrogen atom, the electron emits permanently a stationary matter wave requiring it to stay in the interference fringes of the matter wave with a probability proportional to the intensity of the wave, obtained by solving the Schrödinger equation. The stationary wave exists only for the Bohr values of the energy. The potential energy being function of the position r of the electron, the kinetic energy and thus the velocity v is the difference between the Bohr energy E_n and the electrostatic potential $V(r)$:

$$\frac{1}{2}m_e v^2 = E_n - \frac{1}{4\pi\epsilon_0 r}$$

The equation is undetermined unless one knows either the velocity or the position of the electron. If we use the Bohr values r_n of the orbit, we obtain the velocity for a circular orbit but in the Schrödinger theory, there are no orbits (particle), only orbitals (wave). The Schrödinger equation gives only the wave amplitude, function of the radius. The maximum of the radial probability density, obtained from the wave amplitude, occurs at the Bohr orbit (the Bohr radius).

The hydrogen atom stationary Schrödinger equation (not the time-dependent Schrödinger equation) is three-dimensional, with three degrees of freedom, the radius, the colatitude and the longitude. It is not necessary to solve the radial part of the Schrödinger equation: the energy levels are identical to Bohr's. The spherical part of the Schrödinger equation for the Kepler (central forces) problem is the Laplace equation. It reduces to the Legendre differential equation, whose solutions are the Legendre polynomials, function of the colatitude ϑ . The spherical harmonics are function of both the colatitude ϑ and the longitude φ (see Born 1989, p. 19; Feynman, ch. 19). They are known in many fields of physics like acoustics of spherical bodies (see Dwivedi, p. 58). The spherical harmonics are shown on table 3 in a simplified manner. The nodes are parallels and meridians of a sphere. Their mathematical expression (not normalized) is shown below each drawing. One could say that Schrödinger replaced the Bohr planetary model by the vibrating sun model.

For each ℓ value, there are $(2\ell + 1)$ values of the magnetic quantum number m and of the corresponding orbitals. Multiplying by 2 (due to the Pauli exclusion principle) the number of orbitals gives $2(2\ell + 1)$, the number of electrons in a subshell of the periodic table. One recognizes on table 3 the four ℓ blocks of the

periodic table. Summing again gives the maximum number of electrons in a shell until atomic number $Z = s + (s + p) + (s + p) = 2 + (2 + 6) + (2 + 6) = 18$ (framed), which is the M shell ($n = 3$). For atomic numbers larger than 18, semi-empirical rules have to be used but the periodicity numbers (e.g. the number of electrons in a block) remains those of the spherical harmonics. The periodic table is divided into four blocks named s, p, d, f in the spectroscopic notation, containing respectively 2, 6, 10 and 14 chemical elements.

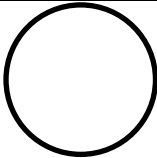
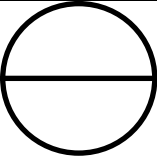
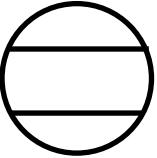
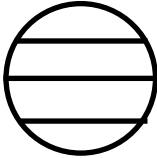
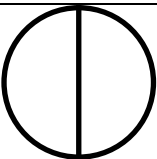
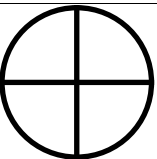
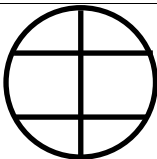
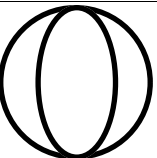
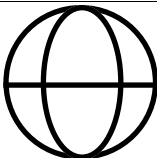
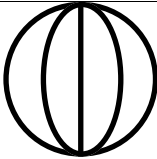
| Table 3: Spherical harmonics | | | | |
|---|--|--|--|---|
| ℓ : secondary or azimuthal quantum number = number of parallels + meridians | | | | |
| m : magnetic quantum number; $ m $: number of meridians | | | | |
| ℓ m | s-block | p-block | d-block | f-block |
| | H, He, alkali metals, alkaline earths | Metals, metalloids, noble gases (without He) | Transition ele- ments (lutetium and lawrencium included) | Lanthanides & actinides (without lutetium and lawrencium) |
| | 0 | 1 | 2 | 3 |
| $m = 0$ |  1 |  $\cos \vartheta$ |  $3 \cos^2 \vartheta - 1$ |  $(5 \cos^2 \vartheta - 3) \cos \vartheta$ |
| $m = \pm 1$ | |  $\sin \vartheta e^{\pm i\varphi}$ |  $\cos \vartheta \sin \vartheta e^{\pm i\varphi}$ |  $(5 \cos^2 \vartheta - 1) \sin \vartheta e^{\pm i\varphi}$ |
| $m = \pm 2$ | | |  $\sin^2 \vartheta e^{\pm 2i\varphi}$ |  $\sin^2 \vartheta \cos \vartheta e^{\pm 2i\varphi}$ |
| $m = \pm 3$ | | | |  $\sin^3 \vartheta e^{\pm 3i\varphi}$ |
| Number of orbitals: $(2\ell + 1)$ | 1 | 3 | 5 | 7 |
| Maximum number of elec- trons or elements in one orbital: $2(2\ell + 1)$ | 2 | 6 | 10 | 14 |
| Maximum number of elec- trons or elements in one atomic shell: $2n^2$ | 2 | 8 | 18 | 32 |
| Subshells in one row of the periodic table | s | s + p | s + p + d | s + p + d + f |

Table 3. The circles (Schaeffer, 2007, p. 169) show the vibration nodes of the angular momentum spheres (Atkins, 2003, p. 5) projected on an axial plane. The azimuthal quantum number ℓ gives the total number of plane nodes and the magnetic quantum number m , the number of meridians. The number of parallels is $(\ell - m)$. The angle ϑ gives the position of the parallels along the vertical z axis and $m \varphi$ the orientation of the meridians. The mathematical expressions of the spherical harmonics are given below the corresponding spheres.

BOHR AUFBAU PRINCIPLE (1921)

The Aufbauprinzip (building-up principle) postulates a hypothetical process in which an atom is progressively "built up" from its predecessor, by adding one proton and one or more neutrons to the nucleus plus one electron to the outermost free atomic orbital. "In eine gänzlich andere neue Richtung wurden diese Bestrebungen später durch das Bohrsche Aufbauprinzip geleitet" (see Pauli, 1979 p. 55, after the Copenhagen conference of October 18, 1921). The Aufbau is similar to building a house, following the blueprint. It is not possible to build the upper floors before the ground floor. The Aufbau is also a form of the principle of minimum energy of natural systems: the added electrons will fall in the lowest energy orbital and then on the existing electrons according to the hydrogen model (the blueprint). If one fills step by step the quantum states of the hydrogen atom with electrons, one obtains the structure of the periodic table up to the atomic number $Z = 18$, e.g. argon. Unfortunately, the theory of the hydrogen atom works only for the atomic numbers smaller than 18. For the higher atomic numbers, specific rules are necessary or, in other words, the blueprint has to be modified for the highest floors of the building.

PAULI EXCLUSION PRINCIPLE (1925)

According to the Pauli exclusion principle, each orbital may contain one or two electrons only (Pauli 1925; see Massimi, 2005, p. 145). Its origin is in spectroscopic and magnetic observations that could be explained only by assuming a quantized intrinsic angular momentum of the electron, called intrinsic spin of the electron, equal to half the hydrogen ground state quantized angular momentum, with only two values, $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$, where $\hbar = h/(2\pi)$ is the reduced Planck constant. The intrinsic magnetic moment of the electron is almost equal to its orbital magnetic moment, the Bohr magneton $\mu_B = e\hbar/(2m_e)$ where e is the electric charge of the electron and m_e its mass.

The exclusion principle may be understood in a simple way. The electron has a magnetic moment like a tiny magnet due to its spinning electrical charge. The magnetic force between magnetic dipoles separated by a distance r varies as $1/r^4$ (Gift, 2009). The electrostatic repulsive force varying as $1/r^2$, the magnetic force is predominant for adjacent electrons. When the magnetic moments are antiparallel, the electrons are attracted. A third electron is not attracted because the resulting magnetic moment is zero. This is the reason why two electrons and only two can be bound when their spins (proportional to their magnetic moment) are opposite.

HUND'S RULE (1925)

Hund's rule of maximum multiplicity (Hund, 1925; see Born 1989, p. 275; Kutzelnigg, 1996) states that the lowest-energy arrangement of electrons in a subshell is obtained by putting electrons into separate orbitals of the subshell with the same spin before pairing electrons. "The observation that among the energy terms associated with a given electron configuration that one is lowest that has (a) the greatest sum of spins and, (b) for terms having the same of spins, the one having the largest sum of orbital angular momenta. The rule allows for exceptions in the case of higher terms" (Mehra, 2000, p. 528).

The orbital defined by the azimuthal quantum number ℓ is progressively filled with $(2\ell + 1)$ electrons having parallel spins until half of the subshell is filled, the magnetic quantum number m varying from $-\ell$ to $+\ell$. The ℓ level is progressively completed until it contains an equal number of electrons with antiparallel spins (see Pauling, 1989, p. 52). Hund's rule is useful to predict the detailed electronic configuration but has no effect on the periodic table structure.

Hund's rule may be interpreted as the reverse of the exclusion principle. Indeed, when the electrons are few, their distance on their orbit is large, the repulsive electrostatic force is thus stronger than the magnetic force. Each electron takes an orientation parallel to the mean magnetic field like a compass in the earth magnetic field. As can be seen with two compasses, the pointers are anti-parallel when they are close and parallel when they are at a distance.

MADELUNG RULE (1926)

The hydrogen atom model ceases to work when $Z > 18$, where an accident occurs, the next sublevel being 4s instead of 3d. According to the Schrödinger theory of the hydrogen atom used to predict the atomic structure of multielectron atoms, we have for argon, a principal quantum number $n = 3$ and an azimuthal quantum number $\ell = 1$. The next element, potassium, should be with the same $n = 3$ and $\ell = 2$ but it is $n = 4$ and $\ell = 0$. This problem is solved by application of Madelung's rule (see Goudsmit, 1964; Madelung, 1953, p. 511; Condon, 1980, p. 516):

1. When consecutive atoms are considered, the electron shells are filled in the order of the sum of two quantum numbers n and ℓ , that is, $(n + \ell)$. With this criterion, the Madelung number is $n + \ell = 5$ for $n = 3$ and $\ell = 2$; it is $n + \ell = 4$ for $n = 4$ and $\ell = 0$. The subshell $4s = 4 + 0 = 4$ appears before $3d = 3 + 2 = 5$, in accord with the increasing order of the Madelung numbers.

2. Shells with equal $(n + \ell)$ numbers are filled in the order of the principal quantum number n , classifying the elements according to $n + \ell$ with the lowest n first. With this criterion, $3d = 3 + 1 = 5$ appears before $4p = 4 + 1 = 5$, is in accord with the increasing order of n .

Table 4 shows the $(n + \ell)$ values for all chemical elements. It can be verified on this table that when $(n + \ell)$ is the same for two successive elements, there is an increase in n . If $(n + \ell)$ is different, there is an increase in ℓ . Exceptions to the rule affect only the electronic structure, not the structure of the periodic table. Table 4 shows the $(n + \ell)$ values for all chemical elements. It can be verified on this table that when $(n + \ell)$ is different for two successive elements, there is an increase in ℓ . If the Madelung number is the same, there is an increase in n .

It is usually assumed that "The electron in the hydrogen atom, in its normal state ($\ell = 0$), does not have any orbital angular momentum, and the picture that we must form of the normal hydrogen atom is accordingly somewhat different from that assumed by Bohr" (Pauling, 1989, p. 33). "The electron is not to be thought of as going around the nucleus, but rather as going in and out, in varying directions, so as to make the electron distribution spherically symmetrical" (Pauling, 1988, p. 125). The problem is that a change in direction of the electron implies an angular momentum. "We can apply in wave mechanics the representation of the angular momentum by a vector diagram, known from Bohr's theory; we therefore here also represent the total angular momentum by a vector ℓ " (Born 1989, p. 143).

The electron having a dual nature, particle and wave, we may resolve the contradiction between the Bohr and Schrödinger theories by adding the quantum angular momenta of the particle, $n \hbar$, according to the Bohr theory, and of the wave, $m \hbar$, according to the Schrödinger theory. The maximal value of the magnetic quantum number m being ℓ , the total angular momentum along the rotational axis would be equal to $(n + \ell) \hbar$.

The angular momentum, having an integer value, may be a simpler clue to the $(n + \ell)$ rule than the energy, provided that the Madelung rule were not coincidental, due to the statistically small number of chemical elements.



















| Table 4: Periodic table with orbitals | | | | | | | | | | | | | |
|---|----------------------------|------------------|------------------|----------|----------|---|---------|---------|---------|-----------------------------|----------|---------------|---|
| According to Schrödinger + Bohr Aufbau + Pauli + Madelung | | | | | | | | | | | | | |
| | | Principal number | Azimuthal number | Subshell | Madelung | Orbitals and associated magnetic quantum number m | | | | Maximal number of electrons | | Atomic number | Chemical elements |
| | | | | | | 0 | ± 1 | ± 2 | ± 3 | Subshell | Row | | |
| Row | Chemical groups | n | ℓ | $n\ell$ | $n+\ell$ | | | | | $2(2\ell+1)$ | $2n^2$ | Z | |
| 1 □ K □ n | H, He | 1 | 0 | 1s | 1 |  | | | | 2 | $2=2n^2$ | 1-2 | H, He |
| 2 □ L □ n | Alkali metals and earths | 2 | 0 | 2s | 2 |  | | | | 2 | | 3-4 | Li, Be |
| | Metalloids, Ne | 2 | 1 | 2p | 3 |  | | | | 6 | $8=2n^2$ | 5-10 | B, C, N, O, F, Ne |
| 3 □ M □ n | Alkali metals and earths | 3 | 0 | 3s | 3 |  | | | | 2 | | 11-12 | Na, Mg |
| | Metalloids, metals, Ar | 3 | 1 | 3p | 4 |  | | | | 6 | $8=2n^2$ | 13-18 | Al, Si, P, S, Cl, Ar |
| 4 | Alkali metals and earths | 4 | 0 | 4s | 4 |  | | | | 2 | | 19-20 | K, Ca |
| | Transition metals | 3 | 2 | 3d | 5 |  | | | | 10 | | 21-30 | Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn |
| | Metalloids, metals, Kr | 4 | 1 | 4p | 5 |  | | | | 6 | 18 | 31-36 | Ga, Ge, As, Se, Br, Kr |
| 5 | Alkali metals and earths | 5 | 0 | 5s | 5 |  | | | | 2 | | 37-38 | Rb, Sr |
| | Transition metals | 4 | 2 | 4d | 6 |  | | | | 10 | | 39-48 | Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd |
| | Metalloids, metals, Xe | 5 | 1 | 5p | 6 |  | | | | 6 | 18 | 49-54 | In, Sn, Sb, Te, I, Xe |
| 6 | Alkali metals and earths | 6 | 0 | 6s | 6 |  | | | | 2 | | 55-56 | Cs, Ba |
| | Lanthanides or rare earths | 4 | 3 | 4f | 7 |  | | | | 14 | | 57-70 | La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb |
| | Transition metals | 5 | 2 | 5d | 7 |  | | | | 10 | | 71-80 | Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg |
| | Metalloids, metals, Rn | 6 | 1 | 6p | 7 |  | | | | 6 | 32 | 81-86 | Tl, Pb, Bi, Po, At, Rn |
| 7 | Alkali metals and earths | 7 | 0 | 7s | 7 |  | | | | 2 | | 87-88 | Fr, Ra |
| | Actinide metals | 5 | 3 | 5f | 8 |  | | | | 14 | | 89-102 | Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No |
| | Transition metals | 6 | 2 | 6d | 8 |  | | | | 10 | | 103-118 | Lr, Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Uub, 113, Uuq, 115... |

Table 4. Periodic system without the detailed electronic structure, replaced by the orbitals. One row of the periodic table, between bold lines, contains one to four subshells. Each sphere represents an orbital with n nodes, spherical and plane. The number of spherical nodes is $n - \ell$. There are $\ell - m$ parallels and m meridians.

For $Z \leq 18$ (argon), rows and shells coincide, the row number is equal to the principal quantum number n in the first column. The second column shows the correspondence with the chemical groups. The next four columns give the principal and azimuthal quantum numbers, their spectroscopic notation and the Madelung number, $n + \ell$. The next four columns show the nodes of the orbitals. Then one finds the number of electrons or elements in each row, given by the formula n^2 , from the spherical resonator, multiplied by 2 from the exclusion principle. It gives the atomic number $Z = 2n^2$ series 2, 8, 18, 32, 50. It differs from the observed series 2, 8, 18, 18, 32 for $Z > 18$ (see Scerri, 1997; see Scerri, 2007, p. 202). Then the hydrogen atomic shells are mixed and n varies through the row. In the last two columns the atomic numbers Z increase top-down with their corresponding chemical elements. Similar "magic numbers", 2, 8, 20, 28, 50, 82, 126 have been found in the atomic nucleus (see Scerri, 2007, p. 263) where the $2n^2$ series is verified for $Z \leq 10$.

| Table 5: Periodic table quantum mechanics consistent | | | | | | | | | | | | | | | | | | | | |
|---|--------------------------------|-------------|--------------------------------|--------------------------------------|--|--|--------------------------------------|--|-------|--------|---|---------|--------------------|----------|-------|-------|-------|-------|-------|-------|
| | s-block | | f-block | | d-block | | | | | | p-block | | | | | | | | | |
| ℓ | 0 | | 3 | | 2 | | | | | | 1 | | | | | | | | | |
| Number of electrons in subshells (impossible to show the anomalies) | | | | | | | | | | | | | | | | | | | | |
| $1, 2 \dots 2(2\ell + 1)$ | 1 | 2 | 1...14 | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 | 2 | 3 | 4 | 5 | 6 |
| Spectroscopic | s^1 | s^2 | $f^1 \dots f^{14}$ | | d^1 | d^2 | d^3 | d^4 | d^5 | d^6 | d^7 | d^8 | d^9 | d^{10} | p^1 | p^2 | p^3 | p^4 | p^5 | p^6 |
| IUPAC groups | 1 | 2 | ? | | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| | 2 elements per block | | 3 nodes: 14 elements per block | | 2 plane nodes (parallels or meridians) 10 elements per block | | | | | | 1 plane node (parallel or meridian): 6 elements per block | | | | | | | | | |
| Row, Period, Shell | Spectroscopic notation $n\ell$ | $m = 0$ | Spectroscopic $n\ell$ | Spectroscopic $n\ell$ $m = 0$ | Spectroscopic $n\ell$ $m = \pm 1$ | Spectroscopic $n\ell$ $m = \pm 2$ | Spectroscopic $n\ell$ $m = 0$ | Spectroscopic $n\ell$ $m = \pm 1$ | | | | | | | | | | | | |
| 1 □ K □ n | 1s | H He | | | | | | | | | | | He | | | | | | | |
| 2 □ L □ n | 2s | Li Be | | | | | | | | | | | 2p B C N O F Ne | | | | | | | |
| 3 □ M □ n | 3s | Na Mg | | | | | | | | | | | 3p Al Si P S Cl Ar | | | | | | | |
| 4 ≈ N | 4s | K Ca | | | | | | | 3d | Sc Ti | V Cr | Mn Fe | Co Ni | Cu Zn | 4p | Ga Ge | As Se | Br Kr | | |
| 5 ≈ O | 5s | Rb Sr | | | | | | | 4d | Y Zr | Nb Mo | Tc Ru | Rh Pd | Ag Cd | 5p | Sn Sn | Sb Te | I Xe | | |
| 6 ≈ P | 6s | Cs Ba | | | | | | | 4f | 57-70 | 5d | Lu Hf | Ta W | Re Os | Ir Pt | Au Hg | 6p | Pb Pb | Bi Po | At Rn |
| 7 ≈ Q | 7s | Fr Ra | 5f | 89-102 | 6d | Lr Rf | Db Sg | Bh Hs | Mt Ds | Rg Uub | 7p | Uut Uuq | Uup Uuh | 117 Uuo | | | | | | |

| Lanthanides and actinides (f-block, $\ell = 3$) | | | | | | | | | | | | | | | |
|---|---------------------------|-------------|-------|-----------------|-------|-------|-----------------|-------|---------------|-----------------|----------|----------|----------|----------|----------|
| 3 plane nodes (parallels or meridians), 14 elements per block | | | | | | | | | | | | | | | |
| | $1, 2 \dots 2(2\ell + 1)$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| | Spectroscopic | f^1 | f^2 | f^3 | f^4 | f^5 | f^6 | f^7 | f^8 | f^9 | f^{10} | f^{11} | f^{12} | f^{13} | f^{14} |
| Row | m $n\ell$ | $m = 0$ | | $m = \pm 1$ | | | $m = \pm 2$ | | | $m = \pm 3$ | | | | | |
| 6 | 4f | La Ce | Pr Nd | Pm Sm | Eu Gd | Tb Dy | Ho Er | Tm Yb | Lr | | | | | | |
| 7 | 5f | Ac Th | Pa U | Np Pu | Am Cm | Bk Cf | Es Fm | Md No | Lr | | | | | | |

Table 5. This periodic table is the usual medium-long form completed with the drawings of the spherical harmonics (the spherical nodes do not show). It is a slightly modified IUPAC table where He is in the s-block instead of the p-block. Lu and Lr are in the d-block instead of the f-block. All blocks have an even number of chemical elements, paired in conformity with the Pauli exclu-

sion principle. The local anomalies of the electronic configuration (the first one appears at chromium, $Z = 24$) are not taken into account. The periods one to three coincide with the hydrogen atomic shells K, L, M ($n = 1, 2, 3$). For the periods 4 to 7 the hydrogen model of the periodic table works only partially. For example, period 6 contains successively the subshells 6s of shell P, 4f of shell N, 5d of shell O, 6p of shell P again.

SUGGESTED UPDATING OF THE COMPACT PERIODIC TABLE

The modified periodic medium long form table 5, IUPAC style, is obtained from table 4. The drawings (Schaeffer, 2007, p. 201) show the spherical harmonics of the atoms outermost orbitals. The subshells are shown in each block and each row in the spectroscopic notation (after Ouahès 1995, p. 109).

The vacant box beside hydrogen is now filled with helium. Lutetium and lawrencium are in the d-block below scandium and yttrium. The lanthanoids and actinoids are 14 each in the f-block as predicted by the exclusion principle and the spherical harmonics. As in most periodic tables, the detailed electronic structure of the atoms does not appear here.

CONCLUSION

There exist a large variety of periodic tables, depending on the criteria used to build them. The physical or chemical properties are innumerable and their choice as a criterion to build the periodic table is subjective. There are also purely mathematical arguments like symmetry criteria but their physical basis is tenuous. The various periodic tables being more than 96 % quantum mechanics consistent, less than four minor corrections are necessary. They consist to place hydrogen, helium, lutetium and lawrencium in their respective ℓ blocks. Helium will be in the s-block and therefore with hydrogen, lutetium and lawrencium in the d-block, below yttrium. It is possible to call He a noble gas of the s-block, Lu and Lr, lanthanides of the d-block. The IUPAC table with these three slight corrections is quantum mechanics consistent.

Tentative explanations of the Aufbau principle, Pauli exclusion principle, Hund's rule and Madelung rule have been given. A geometric representation in the periodic table of all its atomic orbitals allows a quick understanding of its structure based on physics (resonant sphere) and mathematics (spherical harmonics).

REFERENCES

- P.W. Atkins, J. de Paula, Atkins' Physical Chemistry, Oxford University Press, 2002.
 P.W. Atkins, Quanta, Oxford University Press, 2003.
 N. Bartlett, Xenon Hexafluoroplatinate (V) $\text{Xe}^+[\text{PtF}_6]^-$. Proc. Chem. Soc. (June), 218, 1962.
 A. Bent, New Ideas in Chemistry from Fresh Energy for the Periodic Law, Authorhouse, Bloomington, IN, 2006.
 N. Bohr, D. Coster, Z. Phys., 342, 1923a.
 N. Bohr, Nobel lecture, Nature, July 7, 1923b (also in Collected Works ed. by J. R. Nielsen North Holland Amsterdam, Vol. 4, p. 467, 1977).
 M. Born, Atomic Physics, Dover, New York, 1989 (first edition in 1935).
 A.K. Brisdon, Halogens and Noble Gases. Annu. Rep. Prog. Chem., Sect. A, **97**, 107–116, 2001.
 R. Cohen et al, Quantities, units and symbols in physical chemistry, International union of pure and applied chemistry, physical and biophysical chemistry division, Cambridge: Royal Society of Chemistry, 2007.
 E.U. Condon, H. Odabaşı, Atomic structure, Cambridge University Press, 1980.
 L. de Broglie, Annales de Physique - 10e Série - Tome III - Janvier-Février 1925.
 B.N. Dwivedi, Dynamic Sun, Cambridge University Press, 2003.
 U. Fano, L. Fano, Basic physics of atoms and molecules, Wiley, New York, 1959.
 R.P. Feynman, M.L. Sands, R.B. Leighton, The Feynman lectures on physics, Quantum mechanics, California Inst. Techn., 1966.
 E. Fluck, New notations in the periodic table, Pure & App. Chem. 60, 431- 436, 1988.
 S. Gift, Progress in Physics, Vol. 1, p. 12, 2009.
 S.A. Goudsmit, P.I. Richards, Proc. Nat. Acad. Sci. US 51, 664, 1964.

- N.E. Holden, Ty. Coplen, The Periodic Table of the Elements, Chemistry International, **26**, No. 1 January-February 2004.
- F. Hund, Z. Physik, **33**, 345, 1925.
- C. Janet, Concordance de l'arrangement quantique, de base, des électrons planétaires des atomes - avec la classification scalariforme, hélicoïdale, des éléments chimiques, Beauvais - Imprimerie départementale de l'Oise, 1930.
- W.B. Jensen, The Positions of Lanthanum (Actinium) and Lutetium (Lawrencium) in the Periodic Table, Journal of Chemical Education, **59**, p. 634-636, 1982.
- P. Kendall, Heavy elements: A very brief encounter. Nature, **418**, 815-816, 2002.
- J.C. Kotz, K.F. Purcell, Chemistry and chemical reactivity, Saunders College Publ., 1991.
- W. Kutzelnigg, J.D. Morgan III, Hund's rules, the alternating rule, and symmetry holes, Z. Phys. D **36**, 197-214, 1996.
- G.J. Leigh, H.A. Favre, W.V. Metanomski, Principes de nomenclature de la chimie, Introduction aux recommandations de l'IUPAC, De Boeck université, 2001.
- D.A. McQuarrie, P.A. Rock, Chimie générale, De Boeck université, Bruxelles, 1992.
- E. Madelung, Die mathematischen Hilfsmittel des Physikers, Springer-Verlag, 1953 (first edition in 1936).
- M. Massimi, Pauli's exclusion principle, Cambridge University Press, 2005.
- J. Mehra, H. Rechenberg, The historical development of quantum theory, V. 6.1, The completion of quantum mechanics, 1926-1941, Springer, 2000.
- R. Ouahès, C. Ouahès, Chimie physique, Ellipses, Paris, 1995.
- W. Pauli, Z. Physik, **31**, 373, 1925.
- W. Pauli, Wissenschaftlicher Briefwechsel mit Bohr, Einstein, Heisenberg, U.a, Springer, 1979.
- L. Pauling, General Chemistry, Courier Dover Publications, 1988.
- L. Pauling, The Nature of the Chemical Bond and the Structure of Molecules and Crystals, Cornell University Press, 1989 (first edition in 1960).
- E.R. Scerri, Has the periodic table been successfully axiomatized?, Erkenntnis **47**: 229-243, 1997.
- E.R. Scerri, How Good Is the Quantum Mechanical Explanation of the Periodic System?, Journal of Chemical Education, Vol. **75**, No. **11**, 1998a.
- E.R. Scerri, The Evolution of the Periodic System, Scientific American, September, p. 78, 1998b.
- E.R. Scerri, Some aspects of the metaphysics of chemistry and the nature of the elements. HYLE. **11** (1-2), pp. 127-145, 2005.
- B. Schaeffer, Relativités et quanta clarifiés, Publibook, Paris, 2007.
- E. Schrödinger, Ann. d. Physik **79**, 361, 1926.
- P. Strange, A. Svane, W.M. Temmerman, Z. Szotek, H. Winter, Understanding the valence of rare earths from first-principles theory, Nature (London), **399**, 756-758, 1999.
- R.L. Watson, Basic Principles of General Chemistry, Texas A&M University, 2008. cyclotron.tamu.edu/watson/ch101h/Contentsx-103.pdf
- E.H. Wichmann, Quantum physics, Mc Graw Hill, 1971.
- C.G. Wohl, LBNL, The electronic configurations and the ionization energies are from the NIST database, <http://physics.nist.gov>, Reviewed 2005.

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