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Using Atomic Microstates and Atomic Number Parity in Support of Lutetium and Lawrencium Classification as Transition Metals

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Abstract: Unlike other groups of elements, Group 3 constituency remains unsettled. This article argues that ground level microstates and atomic number parity suggest Sc-Y-Lu-Lr Group 3 membership.

Key words: Transition metals, inner transition elements, lawrencium placement, rare earth metals, group 3 constituents, ground level, atomic microstates, atomic number, parity, f-block.

1. The Lu/Lr Problem

Within two or three years, the IUPAC (International Union of Pure and Applied Chemistry) will decide whether lutetium and lawrencium are transition metals that belong to the third group of the periodic table, or in a "footnote" with the rest of the inner transition elements [1].

The periodic law proved to be an excellent instrument for classification of chemical elements that brought us the short form of the periodic table. However, as discoveries that led to the understanding of the atomic structure accumulated, the periodic table underwent another modification and grew from the original 8-group long arrangement to 32-elements long (the long form) that was then shortened to 18-elements long, with a separate 14- or 15-elements long sub-table containing "lanthanides" and "actinides." That sub-table is also called the "f-block" after the spectroscopic term "fundamental". This is where the formulation of the periodic law started to show some cracks. Should the f-block be 14-elements, or 15-elements long? Should the 14-elements long block extend from La(Ac) to Yb(No), or from Ce(Th) to Lu(Lr). Or, in other words, what are the exact limits of the f-block? [2-4].

How can the f-block begin with La and Ac which do not have f-electrons in their outer shells? Moreover, why should lanthanum, which has no f-electrons at all in its ground state, be the first element of the f-block? Following that logic, the f-block should begin with $_{58}$Ce, the atom that features the first electron in the f-orbital, together with $_{90}$Th, which has one f-electron in its outer shell. However, given that there could be only 14 f-orbitals, the f-block should then extend to $_{71}$Lu and $_{103}$Lr. But this is also problematic. Although Lu and Lr have f-orbitals completely filled, quite fitting for the terminal elements of f-block, their valence electrons are s- and d-type, while in $_{70}$Yb and $_{102}$No, which also have f-orbitals filled, one of those f-electrons actually participates in chemical bonds. Furthermore, Sato et al. [5] report that lawrencium's first ionization potential is only 4.96 electron volts, which suggests that Lu and Lr should be the first elements of the third and fourth rows of the d-block, not the f-block.

2. Using Microstates and Atomic Number Parity to Resolve the Problem

In the past, most arguments with regard to

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membership in f-block were based either on chemical behavior, or the energy level of a single (aka differentiating) electron. However, none of the above approaches led to resolution. This is why some decided to promote the 15-element long f-block as a compromise, which flies in the face of quantum theory. I contend that the classification of elements should not be decided on the basis of a single electron, or selected group of electrons. Since an element is a substance that is in essence atoms of the same type, why not look at the properties of whole atoms? Looking at periods, as well as s, p and d-blocks, one can notice that all of them begin with atoms that have odd values of atomic number Z and end with atoms that have even values of Z. Termination of f-block with $_{71}$Lu and $_{103}$Lr that have odd atomic numbers is inconsistent with the rest of the blocks.

Let us explore why periods and blocks should terminate with the elements that have even atomic numbers. The periodic table begins with hydrogen, which has odd atomic number Z = 1. From quantum mechanics we know that the number of electrons in subshells is $(2s + 1)(2l + 1) = 4l + 2$, where s = 1/2 is electron's inherent spin number and l = 0, 1, 2, 3 is the electron orbital angular momentum quantum number. Looking at the periodic table one can notice that each period comprises block rows. Therefore, if blocks of the periodic table are made to reflect electronic subshells s, p, d and f that can hold only even numbers of electrons, the number of elements in each period will always be an even number. Any sequence of natural numbers that has an even number of entries and begins with unity, or any other odd number, will always end with even integer. Therefore, any sequence of natural numbers of length $\sum_{l=0}^{l}(4l + 2)$ that begins an odd number, will always end with an even number. This suggests that every block of the periodic table has to end with elements that have even atomic quantum numbers, which disqualifies $_{71}$Lu and $_{103}$Lr from holding such terminal positions unless, of course, the quantum nature of atoms is completely disregarded.

With regard to orbital filling and electron configurations, such notations as $1s^2 2s^2 2p^6 3s^2$… for example, are not specific enough and do not represent a single state. For example, the electron configuration of cerium is [Xe] $4f^1 5d^1 6s^2$, but there are multiple microstates that have this same configuration and only one of them corresponds to ground level. A major application of f-block elements is in lasers and phosphors, where knowledge of their ground level microstates is essential. Why not use ground level microstates in an attempt to resolve the issues of f-block delineation? (For an overview of microstates, term symbols, etc., see "Quantum Numbers of Multielectron Atoms" in Ref. [6], pp. 41-48.)

Looking at a periodic table that shows ground-state levels of the majority of known atoms [7], it is hard not to notice certain patterns. The periodic table shown in Fig. 1 is in left step format with its blocks ordered in accordance with electron orbital momentum quantum number l = 3, 2, 1, 0 and ground-state level shown for each element. All periods in both, traditional and left step periodic tables, terminate with elements that have the same ground-state level notation: $^1S_0$ meaning that those atoms have all orbitals filled and possess zero total orbital angular momentum (L = 0), as well as zero total angular momentum (J = 0). Their multiplicity values are equal unity (M = 1) which means that total inherent spin of the atoms located at the end of the periods is zero.

It can also be noticed that s, p and d blocks of traditional periodic table and all (s, p, d and f) blocks of the periodic table shown in Fig. 1 terminate with atoms possessing $^1S_0$ ground-state level. The meaning of this is that the elements located at the termination of blocks have all their orbitals completely filled. This does not hold for $_{71}$Lu and $_{103}$Lr, which have ground state levels $^2D_{3/2}$ and $^2P_{1/2}$ respectively meaning that not all their orbitals are closed. This should disqualify them from holding terminal positions in f-block.

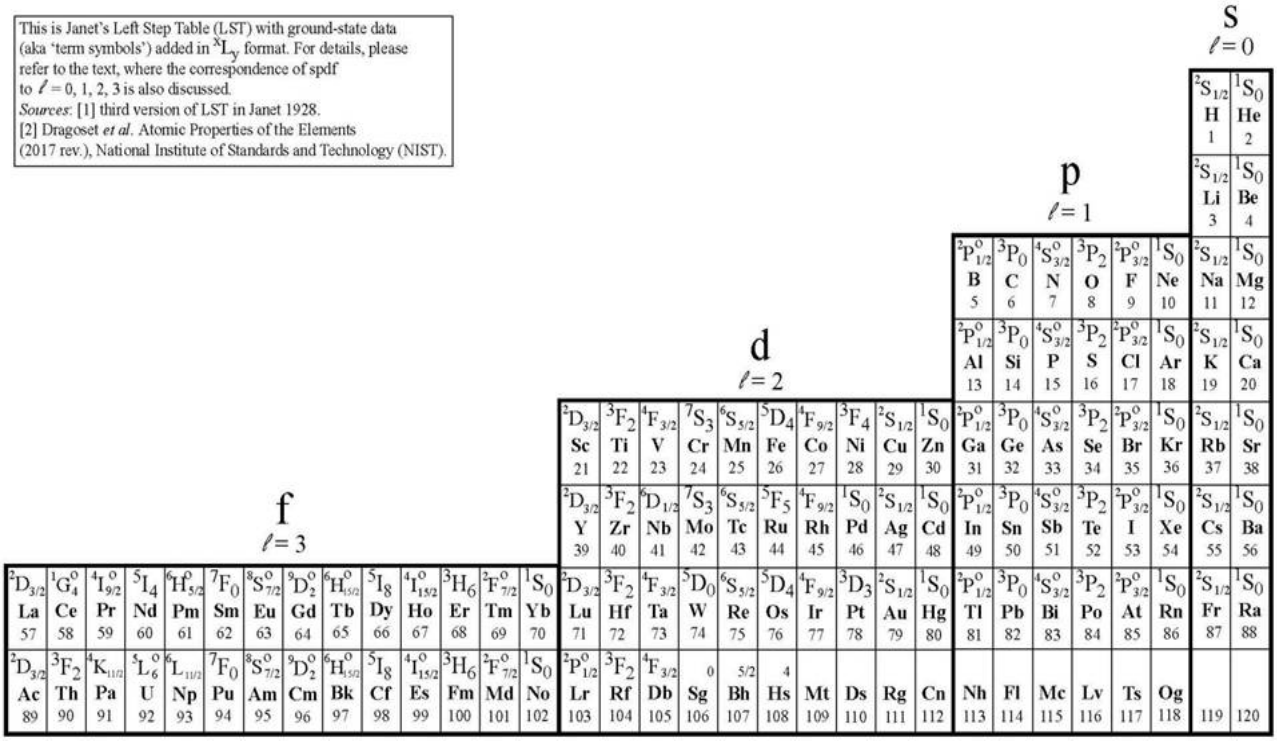

Fig. 1 Annotated left-step table.

Instead, the f-block should terminate with atoms of $_{70}$Yb and $_{102}$No, which both have ground level $^{1}S_{0}$, that is all orbitals in those two atoms are completely filled, including 4f and 5f orbitals. Noting that there could be only fourteen 4f and fourteen 5f orbitals, the conclusion can be made that f-block of the periodic table should begin with $_{57}$La and $_{89}$Ac and terminate with $_{70}$Yb and $_{102}$No. It should also be noted that $_{56}$Ba and $_{88}$Ra, which together mark the termination of the s-block ($^{1}S_{0}$) directly precede $_{57}$La and $_{89}$Ac, respectively, which is another sign that lanthanum and actinium should constitute the beginning of the f-block.

An additional indication that could be used for defining the limits of the f-block is the ground-state levels of the atoms that have half-filled orbitals, such as atoms in groups 1, 7 and 15, or rather 1, 15 and 7, if listed in order of s, p, d (l = 0, 1, 2). Their corresponding ground-state levels are $^{2}S_{1/2}$, $^{4}S_{3/2}$ and $^{6}S_{5/2}$.

It can be extrapolated from the above that atoms with half-filled f-orbitals should have ground-state level $^{8}S_{7/2}$ and, indeed, this is the ground state level that atoms of $_{63}$Eu and $_{95}$Am have, which correlates well with a 14-elements long f-block that starts with $_{57}$La and $_{89}$Ac, and ends with $_{70}$Yb and $_{102}$No.

3. Conclusions

Without resorting to analyzing single electrons, whole atom characteristics such as atomic numbers and ground-state levels can be effectively used to resolve the issue of the Periodic Table's f-block delineation. Note that the periodic table on the inside front cover of Emsley [8] matches this approach exactly. See also page 281 in Emsley, where he explains that Ref. [2] contains the rationale for his unusually formatted periodic table. Here, by a separate line of reasoning, one arrives at the same place: Sc-Y-Lu-Lr, La-Yb, and Ac-No.

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