The Distribution of Atomic Ionization Potentials Reveals an Unexpected Periodic Table

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The experimental distribution of atomic ionization potentials (AIP) reveals an unexpectedly simple atomic structure that disagrees however with the standard atomic model. Quantum mechanics has been unable so far to forecast the first degree equation that governs the distribution of all AIP, and the real order of atomic layers in the periodic table.

We plotted the square root of atomic ionization potential (AIP) available in the literature[1,2,3,4,5,6] with respect to the atomic number Z. Atoms with the same number of electrons N exhibit AIP distributed on the same straight line as visible on figure1.
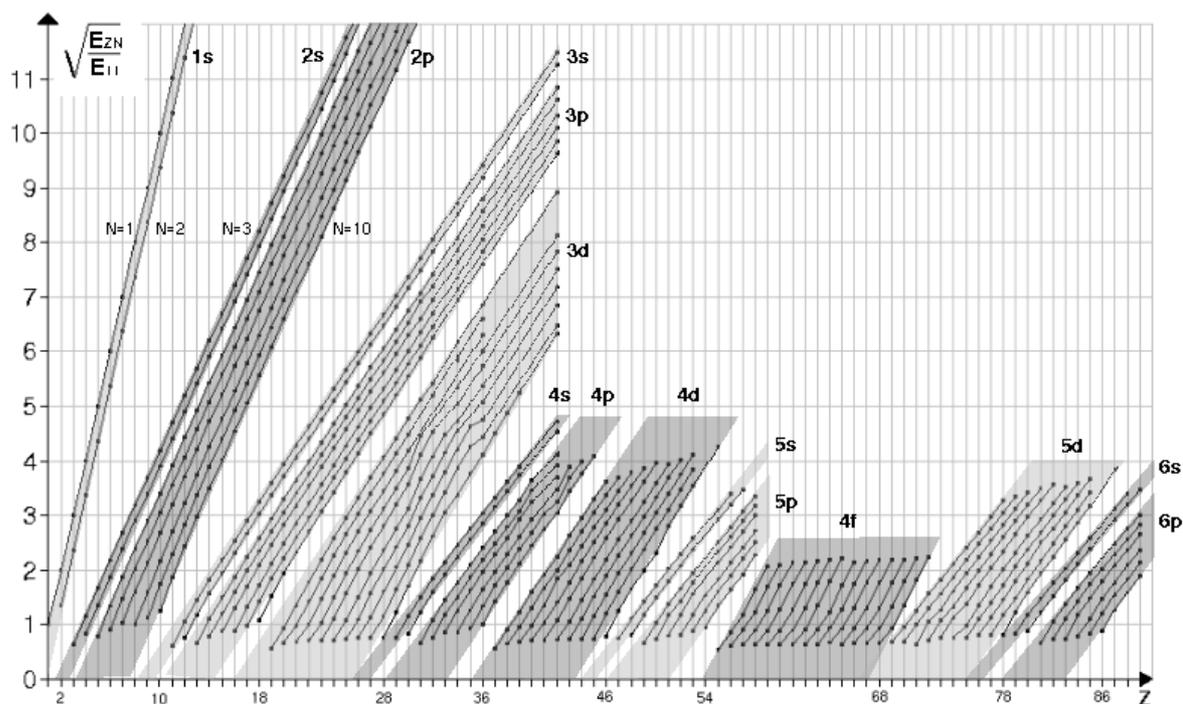

Figure 1 : square root of ionization potentials E_{ZN}, divided by the one of hydrogen E_{11}, with respect to the atomic number Z. N is the number of electrons

in the atom. Lines join the experimental data for each isoelectronic series of atoms, dotted lines in case of interpolation when data is missing between two measures. The different atomic structures are enhanced for a better visibility.

We have no theoretical explanation yet to this distribution of AIP : quantum mechanics did not forecast this atomic property despite its simplicity and its universal character among the periodic table. According to R.P. Feynman[7], the ionization potential represents the most fundamental energy level of atoms but the quantum mechanics is unable to calculate its exact value if there are more than 1 electron. Therefore a simple look at figure 1 makes us wonder why quantum mechanics would be unable to forecast such simple straight lines. But let us first have a closer look to this experimental evidence and its consequences.

The structure of the priodic table shown by figure 1 is rather, but not quite, consistent with the standard atomic model. We can see the expected main electronic layers corresponding to the first quantum number n, and to rows in the periodic table : each one is made of a pack of $2n^2$ parallel straight lines with the same gradient. Furthermore we can observe the sub layers *s* with 2 electrons (i.e. with 2 straight lines), *p* with 6 electrons (i.e. with 6 straight lines) and *d* with 10 electrons (i.e. with 10 straight lines), each one clearly separated energetically from the others. We even see that sub layers *s, p* and *d* are constituted of two equal sub parts.

However, the standard model of atom[7] precise that the sublevel 4s is filled up with electrons before the sublevel 3d, but figure 1 shows the contrary. The same remark can be made for 4d and 5s, and for 5d, 6s and 4f. Actually the order of population of the different atomic layers in the standard model is

1s, 2s, 2p, 3s, 3 p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 5f, 5d, 6p,

but the experimental evidence shows rather

1s, 2s, 2p, 3s, 3 p, 3d, 4s, 4p, 4d, 5s, 5p, 4f, 5d, 6s, 6p.

The consequences of this experimental fact are therefore very important on the shape of the periodic table that should be modified as shown on figure 2. This new view of the periodic table is rather consistent with the chemical properties of elements, but there are however some noticable differences, among them Cu, Ag and Au shall be classified as alcalin metals.

The lines of figure 1 demonstrate that we can calculate the AIP E_{ZN} of an atom, having Z protons and N electrons, with the following formula 1 :

$$E_{ZN} = E_{11} [Z / x - (N-1) / y]^2$$

where **x** and **y** are two constants depending upon N. If n is the first quantum number, the constant x is equal to 1/n for the two first layers, but for the others it oscilates between 0.25 and 0.40. We ran a simulation with the former formula by calculating the square root of AIP for atoms with N<19, and considering that y = n+0.5 : the agreement with the experiment is very good (see table1) despite that this formula is unable to distinguish sub layers *s*, *p* or *d* and of course that it has no theoretical foundation to justify its existence.

We may note that the lines of figure 1 are not absolutely perfect. With no explanation so far on the physical phenomenon producing this "line behavior", we observe however that atoms with a low oxidation state are shifted slightly down the perfect straight line, this shift being maximum for neutral atoms. The reason might be that a part of the ionization energy is given by collisions between atoms when they are not ionic enough to repulse each other efficiently, therefore the measured ionization potential is lowered in proportion.

The challenge is now to find a theoretical explanation to this experimental evidence. The complex mathematical shape of quantum mechanics is in real contrast with the

simplicity of the AIP distribution. Obviously "God does not play dice" with the ionization potentials, at least, and we may wonder if quantum mechanics will be able to explain the AIP measures without some simplifications. All contributions are welcome !

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Figure 2 : the shape of the periodic table indicated by the experimental distribution of atomic ionization potentials.

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Table 1 : Average error for isoelectronic series when using formula 1 to calculate the ionization potentials of atoms with less than 19 electrons.

N	Average calculation error (%)	N	Average calculation error (%)
1	0.13	10	3.19
2	0.58	11	4.87
3	1.08	12	5.4
4	2.47	13	4.94
5	1.64	14	5
6	1.9	15	5.88
7	2.43	16	6.02
8	2.59	17	6.78
9	2.79	18	8