Journal of Science and Technology Vol. 14
ISSN -1605 – 427X
Natural and Medical Sciences (NMS No. 1)
mena@sustech.edu

June /2013

A mathematical Model of Simulated Periodic Table of Elements

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ABSTRACT

The newly mathematical model of atomic structure relates the properties of the parabola to the atoms' shells and orbits. A series of parabolas representing the atom shells, with orbits in a shell equal to the square of shell number, is considered to simulate an element atom. Electrons configuration was developed representing distribution of electrons in orbits of the shells. A new addition of the periodic table of elements based on the electrons configuration was explored. The simulation is very simple and enables to insert new elements to be predicted. The model simulated the recent periodic table in more details. In particular, the transition elements were clearly presented. The periodic table was extended to include additional higher shells. It is an important addition as it opens doors for revealing new symmetries within elements.

المستخلص

في النموذج الرياضي للذرة يرتبط تركيب مدارات وأغلفة الذرة بخصائص القطع المكافئ. تم إدخال التوزيع الإلكتروني من ضمن النموذج، حيث يتم تمثيل توزيع الإلكترونات على المدارات الدائرية في الأغلفة ذات شكل القطع المكافئ. وهذه تعتبر اضافة جديدة تم تقديمها بتمثيل الجدول الدوري للعناصر الكيميائية من خلال نموذج رياضي يجري تنفيذه بواسطة المحاكاة بالحاسوب. المحاكاة المقدمة بسيطة جدا وتمكن من إضافة العناصر الجديدة التي يمكن إكتشافها وعلى الاخص فان العناصر الإنتقالية في الجدول الدوري الحديث تتضح جلياً من النموذج. كما أن الجدول الدوري إمتد ليشمل أغلفة أعلى ومدارات أكثر. ويعتبر النموذج اضافة مهمة تمكّن من إظهار عناصر جديدة في الجدول الدوري ذات خواص مشابهه لعناصر معروفة.

KEYWORDS: periodic table, atom structure, electrons configuration, shell, orbit.

INTRODUCTION

Periodic table symbolizes one such elegant symmetry existing within the atomic structure of chemical elements. Within the atomic structure, this has been widely studied from different prospects, and over the last hundred years different graphical representations of periodic tables have emerged [1]. Each graphical representation of chemical elements attempted to portray certain symmetries in form of columns, raws, spirals, dimensions etc. Out of all the graphical representations, the rectangular form of periodic table, also referred to as long form of periodic table or modern periodic table) has gained wide international acceptance [2]. However, International Union of Pure and Applied Chemistry (IUPAC), does not approve any form as periodic table as a standard form [3].

Prior to Mendeleev's pioneering work in creation of Periodic table, several models were developed. Mendeleev pioneered the work of classifying all the known elements under a periodic law of atomic weights [4]. According to Mendeleev's table, all the elements are represented under a simple tabular format with increasing order of the weights and arranged the elements of analogous nature in columns. Prediction of new elements based on symmetry led to the phenomenal success of graphical representation and opened doors in exploring the symmetries within atomic elements.

In early 20th century, quantum mechanical properties of nature revealed that the number of electrons in an element atom determines its chemical properties rather than atomic weights. Rutherford's formula and Bohr-Balmer formula for the energy levels of hydrogen-like atom (1913) along with other advances in quantum mechanics, led to the design of the modern periodic table with a separate block for transition metals and rare-earth metals [5].

According to Aufbau's principle, electrons should occupy the lower-most electronic sub-shell available. This forms the basis for representation of elements within modern form of periodic table, also referred to as "long form of periodic table". Circular form of periodic table is a newly proposed graphical representation [1]. The aim of this circular form of table is to understand the atomic structure and its properties alongside the periodic table. Recently, the Finite State Machine (FSM) was designed to automate the process of writing down the electron configuration of an atom of any known element attempts to reduce the complexities faced by researchers, scholars and students involved in the field of atomic physics, specifically dealing with the orientation and arrangement of electrons inside the atom and remembering the exceptional trends in the arrangement of electrons inside the orbits, as stated by Parul [6]. This paper presents a mathematical model that simulates the periodic table of the elements based on the newly proposed visualized model of the atomic structure by Fattah (2012). The developed simulation will enable revealing new symmetries within elements.

Model of atomic structure

Fattah in (2012) proposed a visualized mathematical model of atomic structure [7]. Figure 1 (a) represents a simple visualized atom's parabolic shells, represented by a number n, containing the inside orbits. Each parabolic shell n greater than 1, contains an orbit of a unity diameter, atomic unit length, with its centre at the focus of the parabola. At distances from that orbit, in a sequence of 1/4 atomic unit length (a.u.l.) along nucleus axis, the shell contains a number of smaller concentric orbits toward the nucleus (the origin). The capacity of each orbit is two electrons. A section through the y-axis is shown in Figure 1 (b).

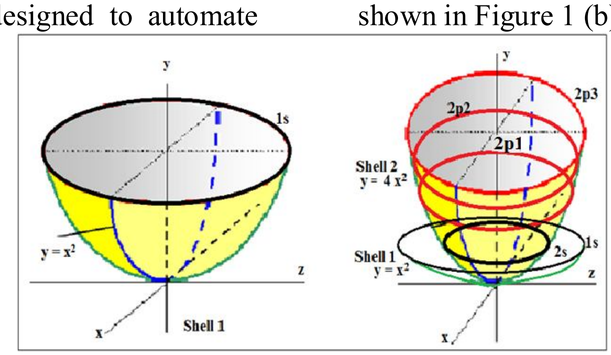

Figure 1 (a): Simple visualized atom's shells

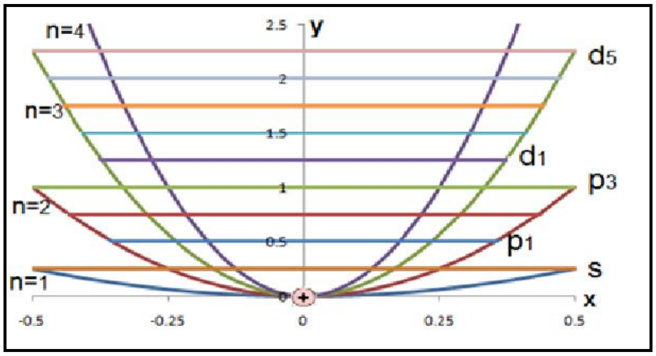

Figure 1 (b): A section through the y-axis

The atom shell equation is given as a parabola:

$$y = n^2 \cdot x^2 \quad \text{...........(1)}$$

where *n* is the number of the shell. Table (1) lists the properties of the shells.

Table 1: Properties of the atom's shells

Shell No. (n)	Shell Equation	Focus (a.u.l.)	Electrons Capacity	No. of Orbits	Types of Orbits in the Shell
1	$y = x^2$	¼	2	1	1s
2	$y = 4x^2$	1	8	4	2s , 2p1-3
3	$y = 9x^2$	9/4	18	9	3s , 3p1-3, 3d1-5
4	$y = 16x^2$	4	32	16	4s , 4p1-3, 4d1-5, 4f1-7
5	$y = 25x^2$	25/4	50	25	5s , 5p1-3, 5d1-5, 5f1-7 , 5g1-9

Electrons configuration

It is noticed that inner shells have more orbits while the outer shell is the widest, with only one orbit. Electrons configuration tells in which orbits the electrons are located. Three rules govern electrons configuration in this model. Firstly, electrons fill orbits starting with lowest shell. Secondly, electrons fill each orbit singly before any orbit of the same type gets a second electron (Hund's Rule). Lastly, orbits are filled in order of Aufbau principle. Electrons are filled in orbits considering that each electron takes its position in its orbit in a certain shell at specific distance from the nucleus.

Journal of Science and Technology Vol. 14
ISSN -1605 – 427X
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June /2013

Shells are divided to right and left to the nucleus. The shells on the left indicate that the specified orbit is complete with two electrons. Electrons in their orbits in the three outer shells are presented in Figure (2).

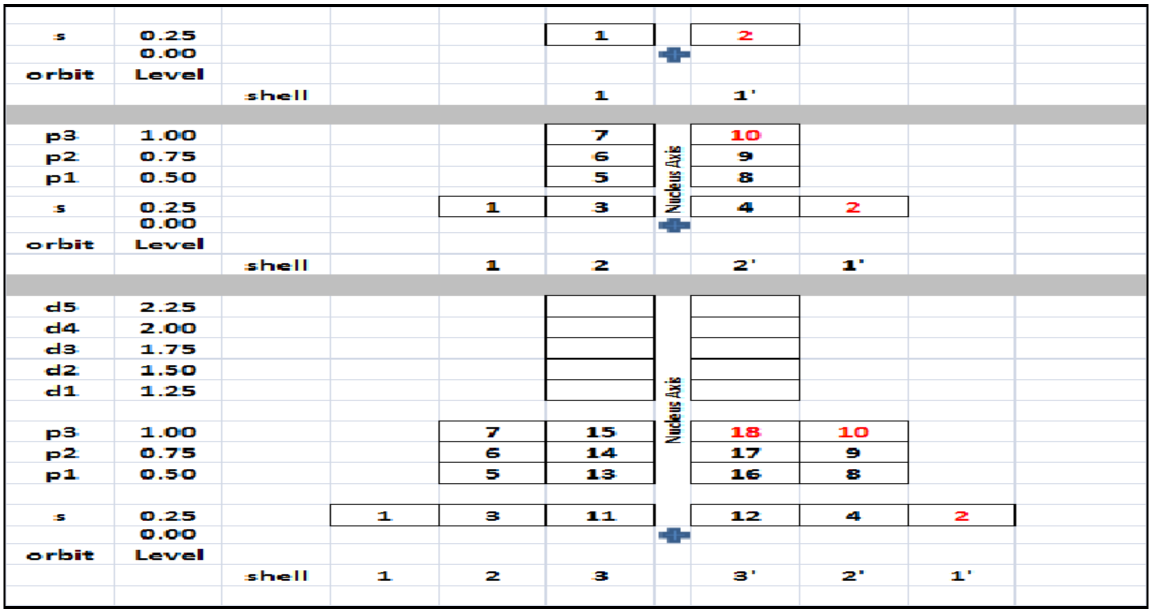

Figure 2: Electrons distribution in the first three shells

The distribution of electrons in four shells and seven shells are presented in Figures 3 and 4, respectively.

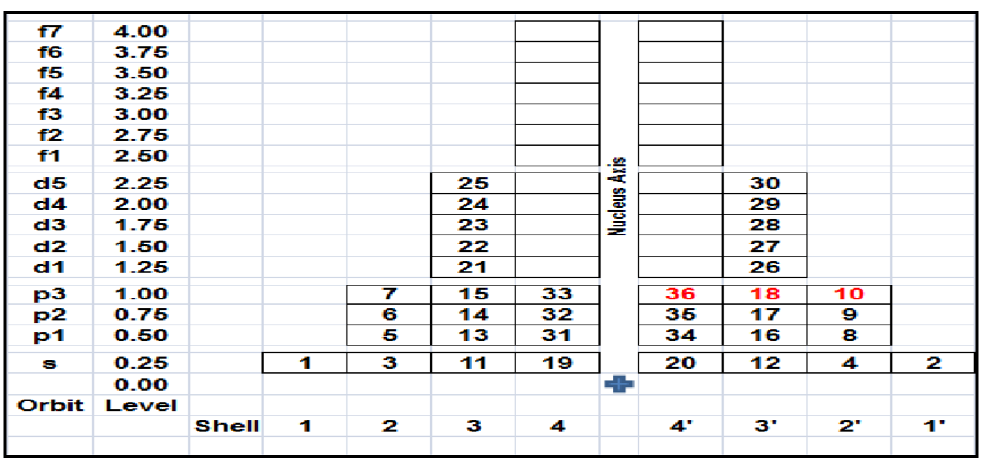

Figure 3: Electrons distribution in four shells

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f7	4.00					63	95						102	70			
f6	3.75					62	94						101	69			
f5	3.50					61	93						100	68			
f4	3.25					60	92						99	67			
f3	3.00					59	91						98	66			
f2	2.75					58	90						97	65			
f1	2.50					57	89						96	64			
d5	2.25				25	43	75	107		Nucleus Axis		112	80	48	30		
d4	2.00				24	42	74	106				111	79	47	29		
d3	1.75				23	41	73	105				110	78	46	28		
d2	1.50				22	40	72	104				109	77	45	27		
d1	1.25				21	39	71	103				108	76	44	26		
p3	1.00			7	15	33	51	83	115		118	86	54	36	18	10	
p2	0.75			6	14	32	50	82	114		117	85	53	35	17	9	
p1	0.50			5	13	31	49	81	113		116	84	52	34	16	8	
s	0.25		1	3	11	19	37	55	87		88	56	38	20	12	4	2
	0.00									+							
Orbit	Level																
		Shell	1	2	3	4	5	6	7		7'	6'	5'	4'	3'	2'	1'

Figure 4: Electrons distribution in seven shells

Obviously, it is noticed that when the p3 – orbits are filled with two electrons, the position of next electron will be in the higher inner shell. Consequently, the core electrons, those are complete in the p3- orbits, represents end of filling the shell. These represent the noble gases elements. In addition, it can also be noticed that the difference in number of electrons for each two successive elements in the noble gases group takes a specific sequence. Table 2 shows these differences and the sequence of the formulae governing it.

Table 2: Differences between no. of electrons in the shells

Shell	1	2	3	4	5	6	7
No. Electrons	2	10	18	36	54	86	118
Difference		8	8	18	18	32	32
Formula		$2*2^2$	$2*2^2$	$2*3^2$	$2*3^2$	$2*4^2$	$2*4^2$

Considering the above derived sequence of this formulae, a new configuration of electrons can be developed. Distribution of electrons in the orbits is traced in Table (3).

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Table 3: Filling orbits in the atom's shells

No. of shells	Types of orbits in shells *													No. of orbits in Shells	No. of filled orbits	No. of empty orbits	No. of electrons in filled orbits
	s	p	d	f	g	h	j	→									
1	1													1	1	0	2
2	2	3												5	5	0	10
3	3	6	5											14	9	5	18
4	4	9	5+5	7										30	18	12	36
5	5	12	10+5	14	9									55	27	28	54
6	6	15	15+5	7+14	18	11								91	43	48	86
7	7	18	20+5	14+14	27	22	13							140	59	81	118
8	8	21	25+5	21+14	9+27	33	26	15						204	84	120	168
9	9	24	30+5	28+14	18+27	44	39	30	17					285	109	176	218
10	10	27	35+5	35+14	27+27	11+44	52	45	34	19				385	145	240	290
11	11	30	40+5	42+14	36+27	22+44	65	60	51	38	21			506	181	325	362
12	12	33	45+5	49+14	45+27	33+44	13+65	75	68	57	42	23		650	230	468	460
13	13	36	50+5	56+14	54+27	44+44	26+65	90	85	76	63	46	25	819	279	540	558

* Orbits filled with two electrons

Figure (5) shows a graphical relation between the number of shells and the number of electrons in the filled orbits.

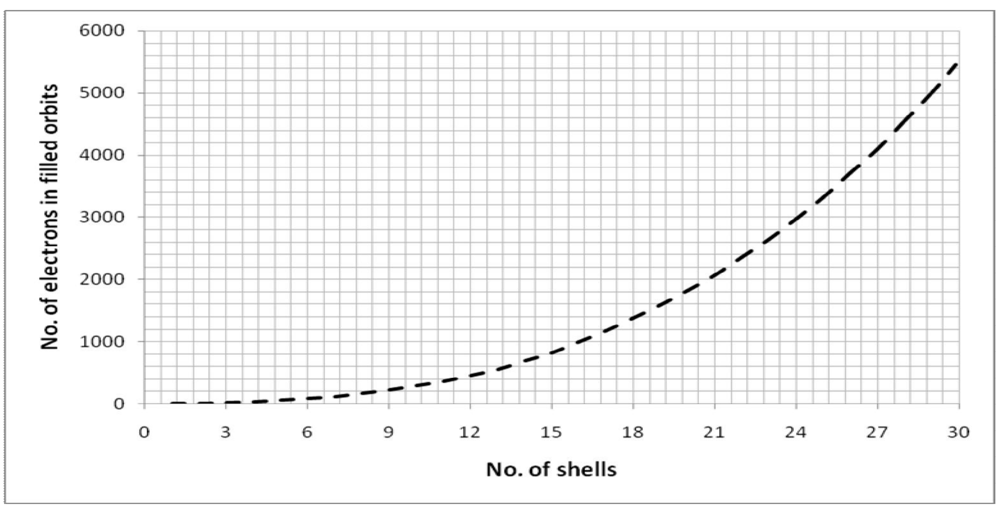

Figure 5: The relation between the number of shells and the number of electrons in the filled orbits

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Modeling of Periodic Table

The periodic table is always constructed along two dimensions: Periods and groups. In this simulation, the periodic table was constructed in accordance to the electrons configuration. The visualized parasailed shape model of atomic structure is the basis of this simulation [7]. The number of electrons of an element specifies the position of the element in the periodic table. In other words, the visualized periodic table locates the elements according to the position of the last electron of an element in the specific orbit in a certain shell.

Figure (6) shows the new invention of the periodic table of the ordinary known elements. The known main groups and the transition elements are presented in a new presentation. Each element, based on electrons number, is located in a specific orbit in its shell.

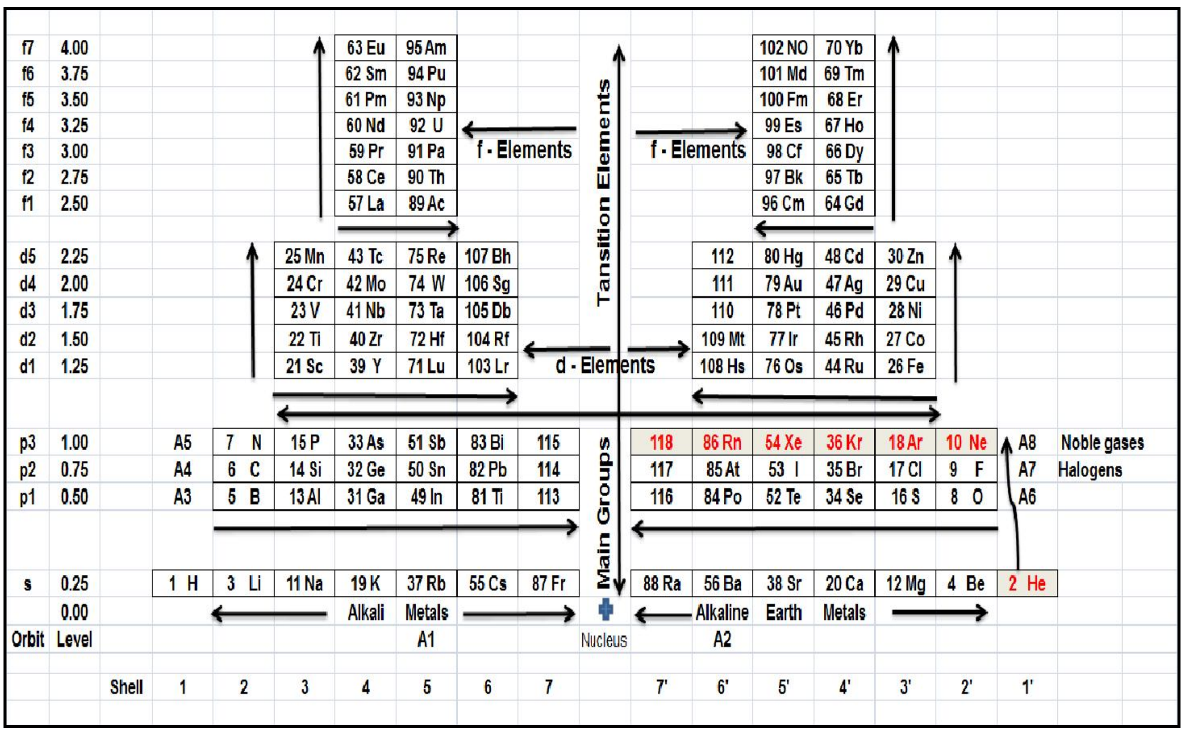

Figure 6: Simulated periodic table (7 Shells)

This model represents a flexible simulation of the periodic table. Simply, inner shells and additional orbits can be inserted. This will enable revealing of new elements and to predict unknown elements of known properties. Figure (7) and Figure (8) represent periodic table of 168 elements in 8 shells and 362 elements in 11 shells, respectively.

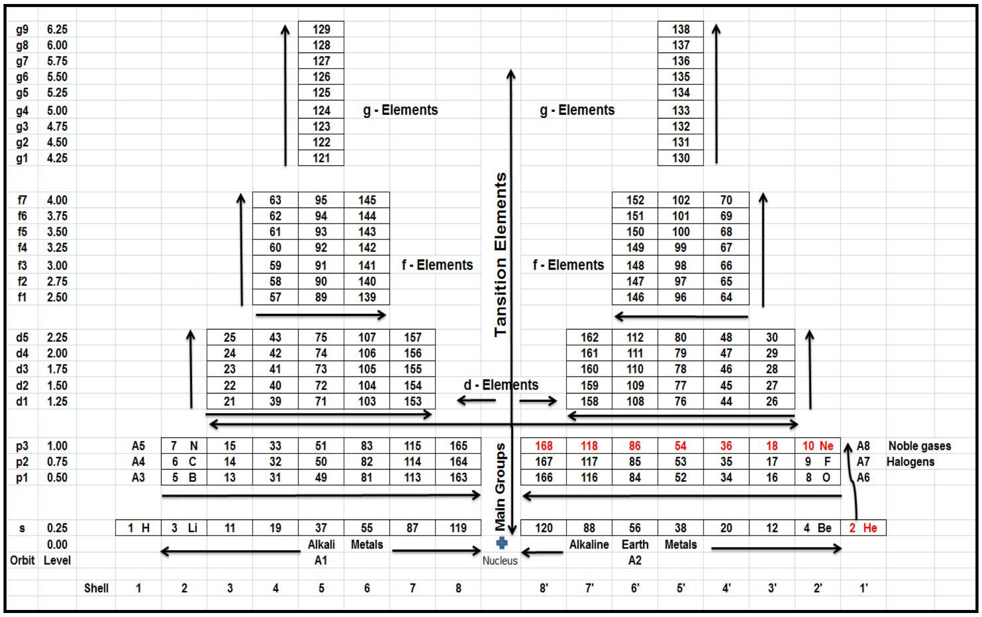

Figure 7: Simulated periodic table (8 shells)

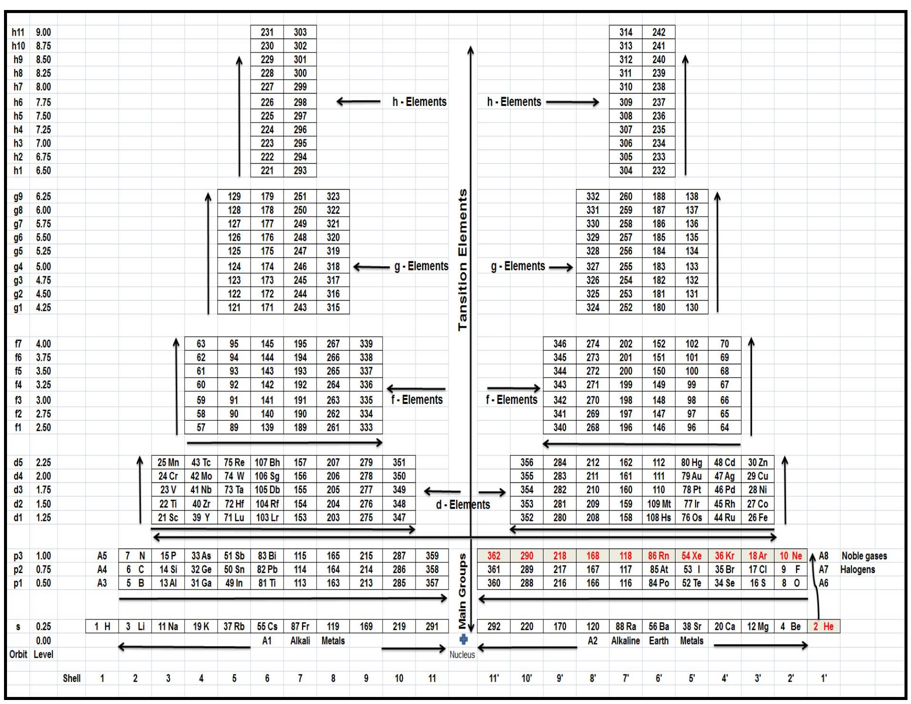

Figure 8: Simulated periodic table (11 shells)

CONCLUSIONS

A mathematical model which simulates electrons configuration was presented. A form of parabolic shells (paraboloids) originating from the nucleus was considered. The outer shell was the first one and the order increases towards the nucleus axis. A new invention of the periodic table of elements based on the electrons configuration was explored. The model simulated the recent periodic table in more details. In particular, the transition elements were clearly presented. The simulation is simple and enables to insert new predicted elements. The periodic table was extended to include higher shells as it opens doors for revealing new symmetries within elements.

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