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Molecular Formula as a Path Using Periodic Table

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Abstract: A molecular formula is a way of expressing information about the proportions of atoms that constitute a particular chemical compound. Using a single line of chemical element symbols. This is the best way to represent any chemical compound. Periodic table in one way has a position in some cell for all the chemical elements based on their atomic numbers. Hexadecimal color codes are used in identifying different colors using color codes. In this paper we propose a method of representing any chemical formula as a path graph using the position of the chemical elements in the periodic table and the colors assigned to them.
Key Words: Molecular formula, chemicals, Periodic Table, Path, Graph, color.

Introduction

Graph theory is extensively used in chemistry. They are used in drawing the structural formula, chem spider representation and so on. It is also used in finding the wiener index, randic index. In [1] the structural formula and Huffmann codes are used to define genetic codes. In [2] dominating set is used in molecular formula encryption.

In this developing society new inventions are part of regular routine and corresponding details of them also happens each day. Many inventions are finally represented using chemical formulas and molecular formulas. In this paper we propose a method representing a chemical formula as a path using periodic table and hexadecimal colors.

Preliminary Note

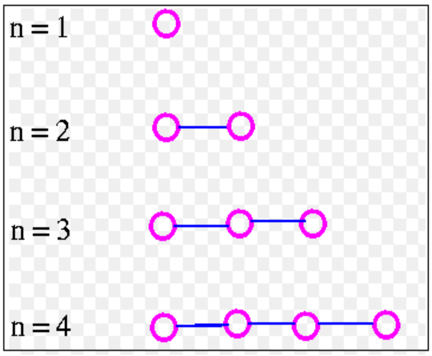
Graph

In a mathematician's terminology, a graph is a collection of points and lines connecting some subset of them. The points of a graph are most commonly known as graph vertices, but may also be called nodes or simply points. Similarly, the lines connecting the vertices of a graph are most commonly known as graph edges, but may also be called arcs or lines [3]. A weighted graph is a graph in which each edge is assigned some numerical value called the weight of the graph.

Path

In graph theory, a path in a graph is a finite or infinite sequence of edges which connect a sequence of vertices which, by most definitions, are all distinct from one another. [4]

A path with n – vertices is denoted by Pn. The following snapshot 1 [5] provides examples of paths with n = 1, 2, 3, 4 vertices.



Snapshot 1

Hexadecimal Colors

Web colors are colors used in designing web pages, and the methods for describing and specifying those colors. Colors may be specified as an RGB triplet or in hexadecimal format. A color is specified according to the intensity of its red, green and blue components, each represented by eight bits. Thus, there are 24 bits used to specify a web color, and 16,777,216 colors that may be so specified. [6]

Materials and Methods

Construction of Color Periodic Table

We choose the usual periodic table. In periodic table colors are used to identify metals, nonmetals etc. We modify the original periodic table by using distinct colors to distinct cells of the table using hexadecimal colors. Except for this, the table looks like the original one. A sample periodic table is given in table 1.

It is seen in table 1 that different colors are used and it resembles the original periodic table. The color codes and the corresponding atomic numbers as used in table 1 is provided in table 2.

Construction of Graph from Color Periodic Table

We use paths for constructing graphs. We consider the molecular formula of the compound. We count the number of elements in the compound (say x). Then we choose a path with x + 1 vertices. We color the edges of the path choosing the color from table in the order in which they appear in the compound. The edges receive weights equal to the number of times each element occurs. For example if the compound is Na_2Cl_3H, then the edge representing Na receives weight 2, the edge representing Cl receives weight 3 and the edge representing H receives weight 1.

Finally we obtain a weighted path with edge colors representing elements. The graph corresponding to Na_2Cl_3H is

Using this method any chemical compound, drug can be represented using their molecular formula. The tree for some examples is provided in table 3. The ball and stick models are from [7]

Table 1

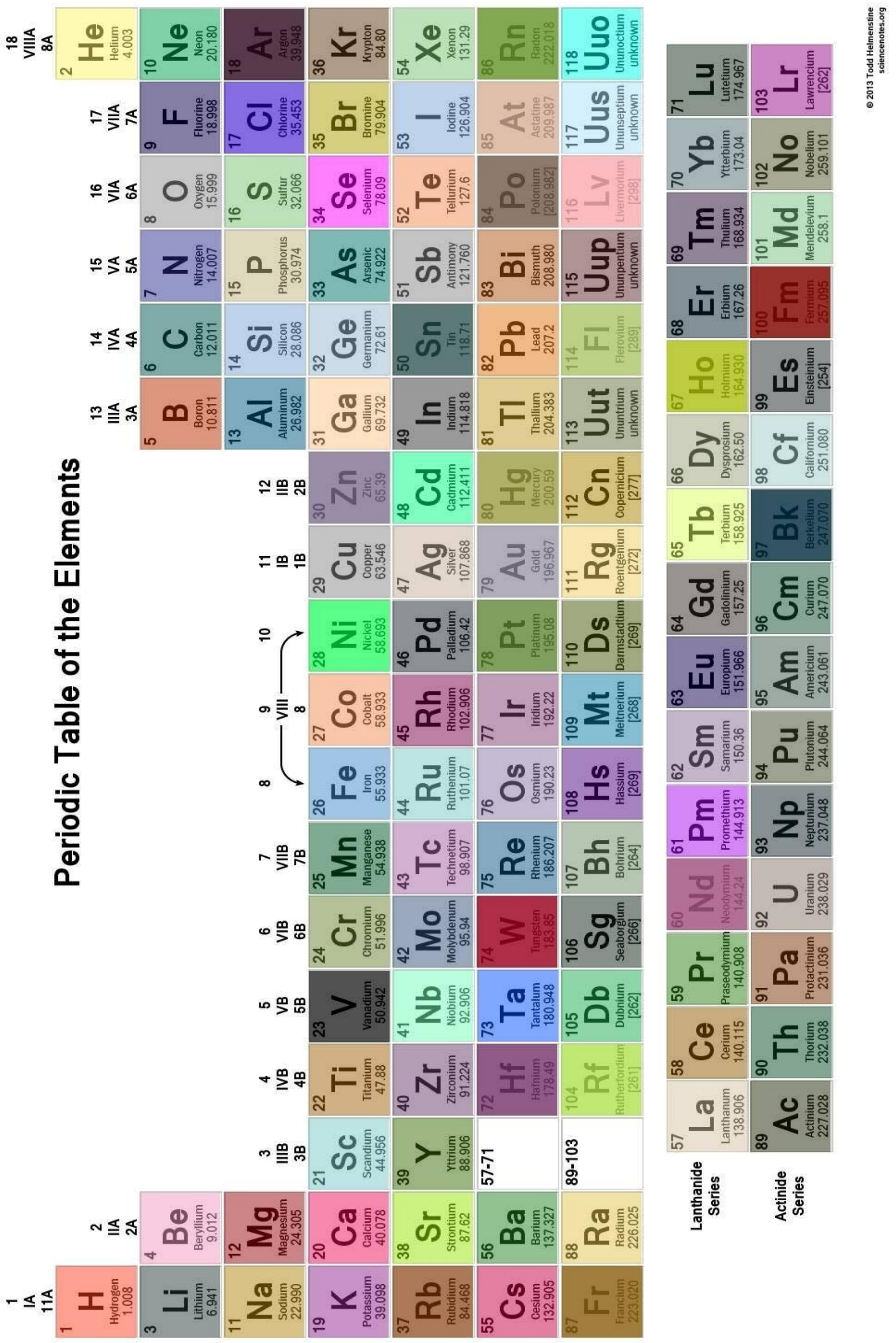

Periodic Table of the Elements
1 IA 1A
2 IIA 2A
3 IIIB 3B
4 IVB 4B
5 VB 5B
6 VIB 6B
7 VIIB 7B
8 9 10 VIII 8
11 IB 1B
12 IIB 2B
13 IIIA 3A
14 IVA 4A
15 VA 5A
16 VIA 6A
17 VIIA 7A
18 VIIIA 8A
1 H Hydrogen 1.008
2 He Helium 4.003
3 Li Lithium 6.941
4 Be Beryllium 9.012
5 B Boron 10.811
6 C Carbon 12.011
7 N Nitrogen 14.007
8 O Oxygen 15.999
9 F Fluorine 18.998
10 Ne Neon 20.180
11 Na Sodium 22.990
12 Mg Magnesium 24.305
13 Al Aluminum 26.982
14 Si Silicon 28.086
15 P Phosphorus 30.974
16 S Sulfur 32.066
17 Cl Chlorine 35.453
18 Ar Argon 39.948
19 K Potassium 39.098
20 Ca Calcium 40.078
21 Sc Scandium 44.956
22 Ti Titanium 47.88
23 V Vanadium 50.942
24 Cr Chromium 51.996
25 Mn Manganese 54.938
26 Fe Iron 55.933
27 Co Cobalt 58.933
28 Ni Nickel 58.693
29 Cu Copper 63.546
30 Zn Zinc 65.39
31 Ga Gallium 69.732
32 Ge Germanium 72.61
33 As Arsenic 74.922
34 Se Selenium 78.09
35 Br Bromine 79.904
36 Kr Krypton 84.80
37 Rb Rubidium 84.468
38 Sr Strontium 87.62
39 Y Yttrium 88.906
40 Zr Zirconium 91.224
41 Nb Niobium 92.906
42 Mo Molybdenum 95.94
43 Tc Technetium 98.907
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.906
46 Pd Palladium 106.42
47 Ag Silver 107.868
48 Cd Cadmium 112.411
49 In Indium 114.818
50 Sn Tin 118.71
51 Sb Antimony 121.760
52 Te Tellurium 127.6
53 I Iodine 126.904
54 Xe Xenon 131.29
55 Cs Cesium 132.905
56 Ba Barium 137.327
57-71
72 Hf Hafnium 178.49
73 Ta Tantalum 180.948
74 W Tungsten 183.85
75 Re Rhenium 186.207
76 Os Osmium 190.23
77 Ir Iridium 192.22
78 Pt Platinum 195.08
79 Au Gold 196.967
80 Hg Mercury 200.59
81 Tl Thallium 204.383
82 Pb Lead 207.2
83 Bi Bismuth 208.980
84 Po Polonium [208.982]
85 At Astatine 209.987
86 Rn Radon 222.018
87 Fr Francium 223.020
88 Ra Radium 226.025
89-103
104 Rf Rutherfordium [261]
105 Db Dubnium [262]
106 Sg Seaborgium [266]
107 Bh Bohrium [264]
108 Hs Hassium [269]
109 Mt Meitnerium [268]
110 Ds Darmstadtium [269]
111 Rg Roentgenium [272]
112 Cn Copernicium [277]
113 Uut Ununtrium unknown
114 Fl Flerovium [289]
115 Uup Ununpentium unknown
116 Lv Livermorium [298]
117 Uus Ununseptium unknown
118 Uuo Ununoctium unknown
Lanthanide Series
57 La Lanthanum 138.906
58 Ce Cerium 140.115
59 Pr Praseodymium 140.908
60 Nd Neodymium 144.24
61 Pm Promethium 144.913
62 Sm Samarium 150.36
63 Eu Europium 151.966
64 Gd Gadolinium 157.25
65 Tb Terbium 158.925
66 Dy Dysprosium 162.50
67 Ho Holmium 164.930
68 Er Erbium 167.26
69 Tm Thulium 168.934
70 Yb Ytterbium 173.04
71 Lu Lutetium 174.967
Actinide Series
89 Ac Actinium 227.028
90 Th Thorium 232.038
91 Pa Protactinium 231.036
92 U Uranium 238.029
93 Np Neptunium 237.048
94 Pu Plutonium 244.064
95 Am Americium 243.061
96 Cm Curium 247.070
97 Bk Berkelium 247.070
98 Cf Californium 251.080
99 Es Einsteinium [254]
100 Fm Fermium 257.095
101 Md Mendelevium 258.1
102 No Nobelium 259.101
103 Lr Lawrencium [262]
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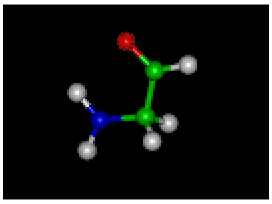
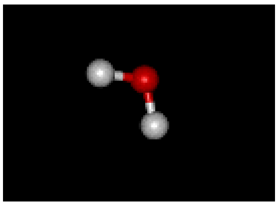
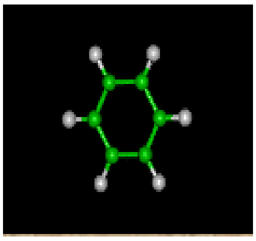
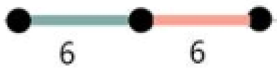
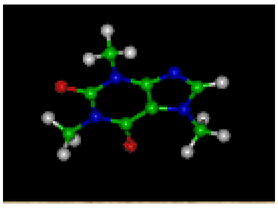
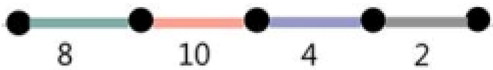
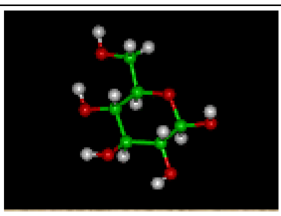
Table 2

1	ffa091	32	9ab9d4	76	c5bcd3	60	a55582
2	fffab3	33	7fb9b5	77	c09fb8	61	d587f6
3	2a3a37	34	ff7fff	78	5e8531	62	c4b7ca
4	f9cce0	35	d5cf7f	79	9590a2	63	877fa3
5	bb3000	36	af9c89	80	9f9e45	64	98948f
6	7faca8	37	833806	81	e2ce92	65	ecfdb0
7	9698c8	38	9ae803	82	f0bb88	66	cdd1be
8	919192	39	396c03	83	d8aa8a	67	acbf0d
9	867fa5	40	b49eb5	84	735a4a	68	849198
10	7fd2a7	41	b8ffdd	85	d6ae94	69	918498
11	b2860e	42	9aa9bb	86	68992e	70	a6b6b9
12	ce8587	43	d3b1d3	87	8e6317	71	8b978f
13	7fadbf	44	bce5e3	88	f0e2a7	89	8f9382
14	bed3ec	45	bd7fa2	89-103		90	83a592
15	c2b67c	46	19252e	104	b0e24f	91	bd9981
16	bce1b9	47	e3d8cc	105	8cd6a6	92	c4bbb5
17	2e08d0	48	00ff84	106	88928c	93	889194
18	300f22	49	9a9a9a	107	b6c6b2	94	9da290
19	c893c7	50	284e4b	108	a783c1	95	9eaba5
20	f689ad	51	c4c4c4	109	86bed2	96	88a698
21	bce5e3	52	fac6aa	110	a2aa81	97	05303e
22	d1b084	53	bed3ec	111	f7e7b0	98	cfe5e3
23	#000000	54	bde2ba	112	d5c27f	99	8d9393
24	6d8332	55	e37fa0	113	b2b99f	100	8.60E+10
25	7fab92	56	92c292	114	adc669	101	bce0c1
26	a1c5e5	57-71	no colour	115	ae9596	102	a8aa94
27	fac6aa	72	77376c	116	fcaeb3	103	cc86c6
28	02fb48	73	7fa9ff	117	d6f1fd		
29	c4c4c4	74	9d0522	118	7ffff4		
30	7c6d8e	75	86aac1	57	ebe2d2		
31	fee2c4			58	c7ad7f		
				59	98c08a		

COLOUR CHART

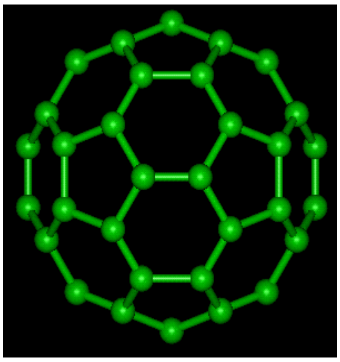
note: lanthanide series: 57-71
Actinide Series: 89-103

Table 3

S. No	Ball and Stick Representation	Molecular Formula	Path
1	 **Glycine**	$C_2H_5NO_2$	
2	 **Water**	H_2O	
3	 Benzene	C_6H_6	
4	 **Caffine**	$C_8H_{10}N_4O_2$	
5	 **d – glucose**	$C_6H_{12}O_6$	

Molecular formula represents the chemical composition of any compound. Any new finding can be encrypted using the method explained. Suppose the received tree is

From table 1 the molecular formula is C_{60} which represents [5]



Fullerene

Now while using colors we observe that some colors look similar but are different. Visually it is tough to find the difference between both colors. This means that looking at the colors and then trying to identify the elements may lead to errors. To avoid this we can include one more weight to the edges which will represent the color codes. The color codes can be converted into smaller numbers and hence used as the weight of the graph. This will improve the representation.

Conclusion

Most of the new inventions like drugs, detergents, etc are finally represented using molecular formula. Communications about these formulas is mandatory and unavoidable. This proposed representation of molecular formula can be used for safe communication of these details. Numerous weighted paths are available in public domain and it is tough to fine the difference between the molecular paths and the usual ones and hence can be used for representing any molecular formula.

Acknowledgment

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References

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