



Technical Note

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Chemical equation as a string using color periodic table

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ABSTRACT

A chemical reaction is best represented as a chemical equation. Any element and its properties are easily identified using periodic table. A wide variety of products we use everyday are developed with the application of chemical reaction. Products like toothpaste, soap, shampoo, cleaning agents etc., are all the results of chemical reactions. Almost all the things around us are made of some kind of substances. New products are always launched in market, and most of them involve chemical equations. Transfer of data regarding them is a must, and safety of the data sent is important for all the industries, due to the heavy competition in today's market. In this paper we propose a method of converting a chemical equation as a string using HTML codes and periodic table.

Key words: chemical equation, molecular formula, colors, HTML code, periodic table.

INTRODUCTION

Today chemistry is doing wonders to mankind and evolving into a branch of science which helps survival at luxury with its never-ending inventions and researches. In the process of growth of new inventions, derivation of new formulas and chemical equations for synthesis of various materials brings in the need of saving and securing the research and hard work from being stolen, copied or being misused while being transferred. In this paper we propose an idea of encrypting the chemical equation using HTML codes.

Various fields of science have contributed to the development of chemistry. In [1] an analysis on the relativity of water resources utilization in Minqin and economic sustainable development is provided. In [2] a comparison of a series of different DFT methods and higher basis sets than the other ones is done in order to find a more suitable method and basis set in predicting geometry and vibration spectra of Pyrimidine adopting optimal multiple regressions. In [3] a simple method of finding the Wiener index of a tree is developed. In [4] a new genetic code is proposed, which can be used for transfer details about DNA sequences. New methods and techniques are developed, which provides scope for development of chemical sciences.

In this paper we propose a method of representing any chemical equation using periodic table and HTML colors as a tool for the same.

Preliminary Note

In this section we provide few discussions used in the encryption of the equation

Periodic Table

The periodic table is a tabular arrangement of the chemical elements, organized on the basis of their atomic number, electron configurations, and recurring chemical properties. Elements are presented in order of increasing atomic number, which is typically listed with the chemical symbol in each box. The standard form of the table consists of a grid of elements laid out in 18 columns and 7 rows, with a double row of elements below that. We use this regular periodic table for our encryption, since elements are best represented using this [5].

Chemical Equation

A chemical equation consists of the chemical formulas of the reactants and the chemical formula of the products. The two are separated by an arrow symbol and each individual substance's chemical formula is separated from others by a plus sign. The stoichiometric coefficients (the numbers in front of the chemical formulas) result from the law of conservation of mass and the law of conservation of charge [6]. We encrypt the regular chemical equation in this paper.

HTML Color Code

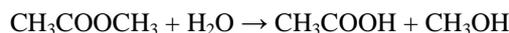
Web colors are colors used in designing web pages, and the methods for describing and specifying those colors. Colors may be specified as an RGB triplet or in hexadecimal format. A color is specified according to the intensity of its red, green and blue components, each represented by eight bits. Thus, there are 24 bits used to specify a web color, and 16, 777, 216 colors that may be so specified. A number of the color swatches below are taken from domain-specific naming schemes such as X11 or HTML4. This html code for colors is used for recognition of a particular shade by the computer, this six bit code is used for the proposed method for encryption [7]. We use this six digit color code for the proposed method.

Proposed String for Chemical Equations

Construction of Color Periodic Table

The first step is to create a new periodic table using HTML colors. In the usual periodic table colors are assigned to represent and classify the elements into different groups. We modify this table and assign different colors to distinct cells of the periodic table randomly. Each cell is represented by a color and each color has a specific color code. So each element in the periodic table is now represented by a color code. A sample periodic table with distinct colors assigned to different cells is provided in Table – 1. Table – 2 provides the color codes assigned to the elements in the periodic table based on the colors used in Table – 1. We have used the base table [8] for preparing the same.

Consider the chemical equation of methyl acetate with water



In chemical equations we notice that an element is prefixed with its stoichiometric index and suffixed with values based on the chemical equation. We convert these values into three digit numbers (This can be converted into numbers of any size depending on the values in the equation). In the above equation the stoichiometric index of C in $\text{CH}_3\text{COOCH}_3$ is 1 and it is not suffixed. So we suffix and prefix C by 001. In H_2O , H has a stoichiometric index 1 and is suffixed by 2. So we suffix H by 001 and prefix it by 002. We replace the elements by the six digit code from table. This is done for each element in the equation. Now + and \rightarrow are replaced with P and E respectively in all places they occur. A chemical equation is now converted into sequence that can be represented as a string of size 3 6 3 3 6 3 with P and E whenever required. This can be summarized in the following algorithm.

Chemical Equation Representation Algorithm

Let S: $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$ be the chemical equation to be encrypted

Step 1: Convert S into a string of numbers, elements, +, \rightarrow in the order in which they appear in the equation (If an element is not suffixed or prefixed by a number replace it by 1, so that each element is prefixed and suffixed by numbers) to obtain S1.

S1: 2H2+1O2 \rightarrow 2H21O1

Step 2: Replace each number in S1 by three digit code (this can vary as per need) to generate S2

S2: 002H002+001O002 \rightarrow 002H002001O001

Step 3: Replace each element by its six digit string from Table to generate S3

S3: 002 ffa091 002+001919192002 \rightarrow 002 ffa091002001919192001

Step 4: Replace + by P and \rightarrow by E to get S4.

S4: 002 ffa091 002P001919192002E002 ffa091002001919192001

Step 5: Send S4 to the receiver.

The procedure is reversed for decryption.

For example suppose the received message is

0067faca8001001919192002
919192006P006919192002.

P006ffa091002001919192001E0017faca8006001ffa091012001

Splitting this into a sequence 3, 3, 6, 3, 3... we generate

Table – 1

Periodic Table of the Elements

18 VIIIA 8A	2 He Helium 4.003	17 VIIA 7A	16 VIA 6A	15 VA 5A	14 IVA 4A	13 IIIA 3A	12 IIB 2B	11 IB 1B	10 VIII 8	9 VIIA 7A	8 VIA 6A	7 VA 5A	6 IVA 4A	5 IIIA 3A	4 IIA 2A	3 IA 1A	18 VIIIA 8A
		9 F Fluorine 18.998	8 O Oxygen 15.999	7 N Nitrogen 14.007	6 C Carbon 12.011	5 B Boron 10.811	4 Be Beryllium 9.012	3 Li Lithium 6.941	2 H Hydrogen 1.008								
	10 Ne Neon 20.180	17 Cl Chlorine 35.453	16 S Sulfur 32.065	15 P Phosphorus 30.974	14 Si Silicon 28.086	13 Al Aluminum 26.982	12 Mg Magnesium 24.305	11 Na Sodium 22.990	10 Ar Argon 39.948								
	36 Kr Krypton 84.80	35 Br Bromine 79.904	34 Se Selenium 78.96	33 As Arsenic 74.922	32 Ge Germanium 72.64	31 Ga Gallium 69.723	30 Zn Zinc 65.39	29 Cu Copper 63.546	28 Ni Nickel 58.693	27 Co Cobalt 58.933	26 Fe Iron 55.845	25 Mn Manganese 54.938	24 Cr Chromium 51.996	23 V Vanadium 50.942	22 Ti Titanium 47.88	21 Sc Scandium 44.956	18 Xe Xenon 131.29
	54 Xe Xenon 131.29	53 I Iodine 126.904	52 Te Tellurium 127.6	51 Sb Antimony 121.760	50 Sn Tin 118.71	49 In Indium 114.818	48 Cd Cadmium 112.411	47 Ag Silver 107.868	46 Pd Palladium 106.42	45 Rh Rhodium 102.906	44 Ru Ruthenium 101.07	43 Tc Technetium 98.907	42 Mo Molybdenum 95.94	41 Nb Niobium 92.906	40 Zr Zirconium 91.224	39 Y Yttrium 88.906	54 Xe Xenon 131.29
	86 Rn Radon 222.018	85 At Astatine 209.987	84 Po Polonium [209]	83 Bi Bismuth 208.980	82 Pb Lead 207.2	81 Tl Thallium 204.383	80 Hg Mercury 200.59	79 Au Gold 196.967	78 Pt Platinum 195.08	77 Ir Iridium 192.22	76 Os Osmium 192.23	75 Re Rhenium 186.207	74 W Tungsten 183.85	73 Ta Tantalum 180.948	72 Hf Hafnium 178.49	71 Rb Rubidium 84.468	54 Xe Xenon 131.29
	118 Uuo Ununoctium [286]	117 Uus Ununseptium [288]	116 Lv Ununhexium [289]	115 Uup Ununpentium [289]	114 Fl Flerovium [289]	113 Uut Ununtrium [289]	112 Cn Copernicium [285]	111 Rg Roentgenium [282]	110 Ds Darmstadtium [285]	109 Mt Meitnerium [288]	108 Hs Hassium [285]	107 Bh Bohrium [284]	106 Sg Seaborgium [286]	105 Db Dubnium [282]	104 Rf Rutherfordium [281]	88 Ra Radium 226.025	54 Xe Xenon 131.29
	71 Lu Lutetium 174.967	70 Yb Ytterbium 173.04	69 Tm Thulium 168.934	68 Er Erbium 167.26	67 Ho Holmium 164.930	66 Dy Dysprosium 162.50	65 Tb Terbium 158.925	64 Gd Gadolinium 157.25	63 Eu Europium 151.966	62 Sm Samarium 150.36	61 Pm Promethium [144.913]	60 Nd Neodymium 144.24	59 Pr Praseodymium 140.908	58 Ce Cerium 140.116	57 La Lanthanum 138.905	88 Ra Radium 226.025	54 Xe Xenon 131.29
	103 Lr Lawrencium [262]	102 No Nobelium 259.101	101 Md Mendelevium 258.1	100 Fm Fermium 257.092	99 Es Einsteinium [254]	98 Cf Californium 251.080	97 Bk Berkelium 247.070	96 Cm Curium 247.070	95 Am Americium 243.061	94 Pu Plutonium 244.064	93 Np Neptunium 237.048	92 U Uranium 238.029	91 Pa Protactinium 231.036	90 Th Thorium 232.038	89 Ac Actinium 227.028	88 Ra Radium 226.025	54 Xe Xenon 131.29

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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	72	8f9382
14	bed3ec	45	bd7fa2	89-103		73	83a592
15	c2b67c	46	19252e	104	b0e24f	74	bd9981
16	bce1b9	47	e3d8cc	105	8cd6a6	75	c4bbb5
17	2e08d0	48	00ff84	106	88928c	76	889194
18	300f22	49	9a9a9a	107	b6c6b2	77	9da290
19	c893c7	50	284e4b	108	a783c1	78	9eaba5
20	f689ad	51	c4c4c4	109	86bed2	79	88a698
21	bce5e3	52	fac6aa	110	a2aa81	80	05303e
22	d1b084	53	bed3ec	111	f7e7b0	81	cfe5e3
23	#000000	54	bde2ba	112	d5c27f	82	8d9393
24	6d8332	55	e37fa0	113	b2b99f	83	8.60E+10
25	7fab92	56	92c292	114	adc669	84	bce0c1
26	a1c5e5	57-71	no colour	115	ae9596	85	a8aa94
27	fac6aa	72	77376c	116	fcaeb3	86	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

006 7faca8 001 001 919192 002 P 006 ffa091 002 001 919192 001 E 001 7faca8 006
 001 ffa091 012 001 919192 006 P 006 919192 002.

From Table – 2 the strings of size 6 represent the following

7faca8: Code for C

ffa091 : Code for H

919192: Code for O

Replacing the three bit strings by their corresponding decimal values we generate the following
 6C1O2P6H21O1EP1C61H121O2P6O2

The decrypted message represents photosynthesis [9]

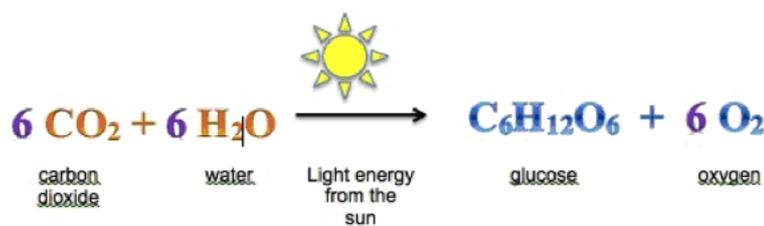


Table – 3 represents few chemical reactions and their encryption codes [10] [11].

S. No	Chemical Equations and their Encryptions
1	<div style="text-align: center;"> <p> $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ methane oxygen carbon dioxide water </p> </div> <p style="text-align: center;">0017faca8001001ffa091004P002919192002E0017faca8001001919192002P002ffa091002001919192001.</p>
2	<div style="text-align: center;"> <p> $\text{CaCl}_2 + 2\text{NaHCO}_3 \rightarrow \text{CaCO}_3 + 2\text{NaCl} + \text{H}_2\text{O} + \text{CO}_2$ calcium chloride sodium bicarbonate calcium carbonate sodium chloride water carbon dioxide </p> </div> <p style="text-align: center;">001f698ad0010012e08d0002P002b2860e001001ffa0910010017faca8001001919192003E001f698ad7faca8001001919192003P002b2860e0010012e08d0001P001ffa0910020019191920017faca8001001919192002.</p>
3	<div style="text-align: center;"> <p> Reactants Products $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} + \text{Energy}$ Hydrogen Oxygen Water </p> </div> <p style="text-align: center;">002ffa091002P001919192002E002ffa091002001919192001.</p>
4	<div style="text-align: center;"> <p> $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ </p> </div> <p style="text-align: center;">0017faca8001001ffa091004P002919192002E0017faca8001001919192002P002ffa091002001919192001.</p>

Table – 3

CONCLUSION

In the present scenario chemistry is ever evolving and developing. This proposed method helps in a double encryption which is almost impossible to decode without the key because of the following reasons which helps in safe and secure information transmission.

- The array is complicated and in itself without decoding has no meaning.
- The array fragmentation needs to be done in a specific order. If fragmentation pattern is not followed then the generated array becomes tougher to decode.
- In case of wrong selection the array can be arranged in thousand of possible / desired combinations, which leads the search in a wrong direction, creating time wastage in computation of wrong code, causing misleading by their own trusted systems for example
002ffa091002P001 919192002E002ffa091002001919192001 can be de fragmented in the following wrong combination
 - 002f fa091002 P001 9191920 02E002ffa 09100200 1919192001.
 - 002f fa0 91002P00 1 919192002E00 2ffa0910 0200191919200 1.
 - 002f fa09 1002P 0019 19192 002E0 02ffa09 100200 1919 1920 01...
- The fragmented array in itself is encrypted. As the 6 sized array is a code of the color.
- The guessing of the color becomes difficult because of 16,777,216 color possibilities. With the probability of guess

$$P(\text{correct_guess}) = 1 / 16,777,16 \\ = 5.9960 \times 10^{-9}$$

- Even at correct guessing the color code with a probability of order -9, the chosen color should again be chosen, as it represents an element out of 118. Once the code is found, for the code as it could be of any of 118 elements. The next code would belong to an element of 117 rest of elements, hence

$$\text{Permutations of the finding HTML} = 118_{\text{first element}} \times 117_{\text{second element}} \times 116_{\text{third element}} \times \dots \times 2_{117\text{th element}} \times 1_{118\text{th element}} \\ = 118! = 4.684526e+194$$

So, with this new way of representation of chemical research can help us in protecting the data using the key, keeps the data secure and safe between the sender and the receiver preventing misuse and piracy of the data.

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