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QUANTUM ANALYSIS OF THE EFFECT OF ERYTHRITOL VS. THE NITROGENATED BASES OF DNA AND RNA CONSTRUCTION

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ABSTRACT

Erythritol (ETT) ((2R, 3S) -butane-1, 2, 3, 4-tetraol) is a polyalcohol (sugar alcohol) used as a substitute for sweet flavors. The present work shows the theoretical quantum analysis to calculate the effect of ETT on the nitrogenous bases (NB) of the nucleic acids (DNA-RNA). The combination of the compound ETT with the DNA and RNA bases was calculated with the Electron Transfer Coefficient (ETC) theory and design in Hyperchem software. SE-PM3 was the specific program used for molecular modeling HOMO-LUMO, BG, EP, and other properties. The water has the highest ETC value of all. For this reason, water can attack the other seven substances in question; but the ETT has a considerable attack power too (it is no good). We calculated ETCs values of the substances in the crossed band, and it can see that the ETT interacts with all NB in oxidative form. It is, in general, concluded that: ETT is an oxidizing agent of both DNA and RNA and due to its average probability the damage it can cause is slow. It is not fulminating.

INTRODUCTION

ETT ((2R, 3S) -butane-1, 2, 3, 4-tetraol) is a polyalcohol (sugar alcohol) used as a substitute for sweet flavors. It has been approved in the United States as a sweetener, as well as in some other parts of the world. It occurs naturally in fruits and fermented foods. ETT is natural alcohol (polyol) sugar present in certain fruits and products derived from the fermentation of wine, soy, and cheese. Its molecular formula is C5H10O4, and its molecular weight is 122.12 g / mol. It is the first industrially manufactured polyol, where the glucose passes a fermentation process by Aureobasidum sp, until generating ETT. [1, 2]

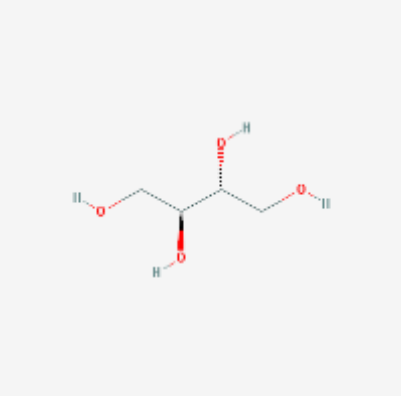

Figure 1. PubChem CID: 222285 Chemical Names: ERYTHRITOL; Meso-Erythritol; 149-32-6; Erythrol; Phycitol; ((2R, 3S)-butano-1, 2, 3, 4-tetraol).

ETT is rapidly absorbed by the small intestine, so it is not metabolized by the body and therefore is excreted in the urine. [3]

ETT has a sweetening power of 70% to 80% compared to that of sucrose and is considered non-caloric due to its low energy content of 0.2 kcal / g. It presents good physical-chemical stability, since it does not react with other active ingredients, it resists storage and remains intact at extreme temperature changes (160 ° C), it is stable in pH ranges of 2-10.2, and it develops synergism with high-quality-sweeteners-power. It does not alter the levels of glucose or insulin so it comes to consider an appropriate substitute for diabetics. Due to its resemblance to sucrose in flavor, appearance and crystallinity, ETT is also used in tabletop sweeteners, but without adding calories. [4] The non-acidogenicity of polyols such as ETT has been demonstrated, since it does not alter the pH of the plaque, creating an environment that is not suitable for the formation of bacteria that demineralize the dentin, for which reason it is attributed with very low cariogenic capacity. [4]

It has been shown to be an excellent radical eliminating polyol, so it has uses as an antioxidant in vivo, since it provides protection against vascular damage induced by hyperglycemia. [5]

Some safety studies have shown that ETT is well tolerated in the human body without causing toxicological effects. In the United States, WHO has granted the name of "unspecified" daily consumption, through the expert committee on food additives of the food and agriculture organization? [6]

Some research shows that humans do not have enzymes that break down ETT. It is absorbed into the bloodstream and excreted unchanged through the urine. When healthy people consume ETT, there is no change in blood sugar or insulin levels. There is also no effect on cholesterol, triglycerides or other biomarkers. [7]

The ETC theory

The BG is defined as the energy difference between the valence band and the conduction band. In the BG there are no electronic states available; this means that when an electric field is applied the electrons cannot increase their energy. [8]

In quantum theory, it is known as HOMO and LUMO, and in the old theory they are known as E- and E +. The LUMO is defined as the range of electric energy that allows acceleration in electrons by the presence of electrical currents and is also called conduction band; HOMO is defined as the highest energy interval that is occupied by electrons in absolute zero value and is called valence band. The HOMO is the most electron-filled orbital, while the LUMO is the orbital that lacks electrons. The HOMO equaled to zero (HOMO 0) is the last layer full of orbitals meaning that it is in the last valence orbital. The LUMO equaled to zero (LUMO 0) is the last layer that lacks electrons.

EP is defined as the total potential energy of the molecule. It is an electrostatic field vector that is defined as the potential that the electron needs to jump the Bohr radius (0.53 Armstrong) by its calculated natural electromotive force (EMF). The negative E value (E-) is the electrostatic potential with negative poles, while the positive E value (E +) is the proton-electron potential [6]. The EP, in other words, means that having 1 EP is having 1 volt for Armstrong. The EP is obtained by the absolute difference of E- and E +.

The ETC is defined as the dimensionless parameter that describes an electrochemical reaction, which is interpreted as the number of times the potential energy needs to jump to the BG. It is calculated by dividing the BG and the EP entirely. That is, if it has a BG of 10 and an ETC of 40, it means that you need 40 times the EP value in EV so that the BG of 10 jumps from the HOMO to LUMO. [9-11]

MATERIALS AND METHODS

SE-PM3 is a program for molecular modeling used by scientists to analyze the quantum composition of molecules for HOMO-LUMO, BG, EP, and other properties. These data are used to form the table where is the ETC´s of the interaction between the ETT and the NB. The Software Hyperchem Professional performs Molecular modeling and analysis of the Lev and the NB. (Hyperchem, hypercube, Multi in for Windows, series 12-800-1501800080.) (Multi in South 1236-301 Tlacoquemecatl Insurgentes Col. del Valle, Benito Juárez, DF, Mexico C.P. 03200).

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The values are obtained from the simulation of molecules of the compounds in the HYPERCHEM software. The software calculates the band gap, the potential energy, and data of the energy transfer coefficient (for its acronym in English, BG, EP, ETC). When designing the molecule, it obtains the values of E- and E + (HOMO-LUMO) in value at zero and a density of 0.015. The crossed compounds of the bands are taking the values of the initial calculation and exchanging it with another compound of interest. The lowest value of ETC is the one of interest as the most reactive compound.

Table 1. Parameters used for quantum computing molecular orbitals: HUMO and LUMO

Parameter	Value	Parameter	Value
Total charge	0	Polarizability	Not
Spin Multiplicity	1	Geometry Optimization algorithm	Polak-Ribiere (Conjugate Gradient)
Spin Pairing	RHF	Termination condition RMS gradient of	0.1 Kcal/Amol
State Lowest Convergent Limit	0.01	Termination condition or	1000 maximum cycles
Interaction Limit	50	Termination condition or	In vacuo
Accelerate Convergence	Yes	Screen refresh period	1 cycle

Table 2. Parameters used for visualize the map of the electrostatic potential of the molecules

Parameter	Value	Parameter	Value
Molecular Property	Property Electrostatic Potential	Contour Grid increment	0.05
Representation	3D Mapped Isosurface	Mapped Function Options	Default
Isosurface Grid: Grid Mesh Size	Coarse	Transparency level	A criteria
Isosurface Grid: Grid Layout	Default	Isosurface Rendering: Total charge density contour value	0.015
Contour Grid: Starting Value	Default	Rendering Wire Mesh	

RESULTS AND DISCUSSION

Quantum interactions of pure substances

In table 1, it can see the water has the highest ETC value of all. For this reason, water can attack the other seven substances in question; but the ETT has a tremendous attack power due to the value of its ETC (second in table 1).

Table 3. ETCs values of the compounds to be analyzed.

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	Water	Water	-12.316	4.059	16.375	-0.127	0.171	0.298	54.95
2	ETT	ETT	-11.661	1.477	13.138	-0.078	0.183	0.261	50.337
3	Thymine	Thymine	-9.441	-0.475	8.966	-0.123	0.169	0.292	30.707
4	Uracil 1	Uracil 1	-9.71	-0.511	9.2	-0.126	0.171	0.297	30.975
5	Uracil 2	Uracil 2	-9.91	-0.415	9.495	-0.147	0.202	0.349	27.208
6	Cytosine	Cytosine	-9.142	-0.344	8.799	-0.174	0.161	0.335	26.265
7	Adenine	Adenine	-8.654	-0.213	8.441	-0.14	0.156	0.296	28.518
8	Guanine	Guanine	-8.537	-0.206	8.331	-0.15	0.172	0.322	25.872

The guanine-guanine attraction has the smallest value of the ETCs in the table. Therefore, this attraction is the most stable of all.

The attack of the water on the nitrogenous bases are fundamental because this is the source of life; intervenes in all metabolic processes.

Quantum interactions of substances in crossed-band

Table 2 shows the ETCs values of the substances in a crossed band. In this table, we can see that the ETT interacts with all nitrogenous bases in oxidative form.

Table 4. ETCs values of substances in crossed bands with ETT

N	Reducing agent	Oxidizing agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	ETT	Water	-11.661	4.059	15.720	-0.078	0.171	0.249	63.133
2	ETT	ETT	-11.661	1.477	13.138	-0.078	0.183	0.261	50.337
3	ETT	Adenine	-11.661	-0.213	11.448	-0.078	0.156	0.234	48.923
4	ETT	Cytosine	-11.661	-0.344	11.317	-0.078	0.161	0.239	47.351
5	ETT	Guanine	-11.661	-0.206	11.455	-0.078	0.172	0.250	45.820
6	ETT	Thymine	-11.661	-0.475	11.186	-0.078	0.169	0.247	45.287
7	ETT	Uracil 1	-11.661	-0.511	11.150	-0.078	0.171	0.249	44.779
8	Water	ETT	-12.316	1.477	13.793	-0.127	0.183	0.310	44.494
9	ETT	Uracil 2	-11.661	-0.415	11.246	-0.078	0.202	0.280	40.164
10	Uracil 1	ETT*	-9.710	1.477	11.187	-0.126	0.183	0.309	36.204
11	Thymine	ETT*	-9.441	1.477	10.918	-0.123	0.183	0.306	35.680
12	Uracil 2	ETT*	-9.910	1.477	11.387	-0.147	0.183	0.330	34.506
13	Adenine	ETT*	-8.654	1.477	10.131	-0.140	0.183	0.323	31.365
14	Guanine	ETT*	-8.537	1.477	10.014	-0.150	0.183	0.333	30.072
15	Cytosine	ETT*	-9.142	1.477	10.619	-0.174	0.183	0.357	29.745

** The ETT behaves as an oxidizing agent of four of the essential bases. The uracil in its two tautomeric forms (U1 = Ketone oxygen; and U2 = alcoholic oxygen)*

Specifically, the six interactions shown with an asterisk in the table are the lowest of all the ETCs. These values indicate that ETT is a very oxidative agent for all nitrogenous bases. Therefore, the ETT can be harmful to both DNA and RNA.

Figure 2 shows the quantum well of the Cytosine - ETT interaction. The ETC is of this quantum well is the minimum and therefore the most likely to be carried out.

In this figure 2, the dotted lines represent the ETCs values of the two pure substances that are being combined. The green dot indicates the reduction and the red dot the oxidation.

It was agreed that the order of oxidation and reduction is as follows: Reducing agent (left side) – Oxidizing agent (right side).

The asterisk interactions in table 4 (from 10 to 15) present a similar pattern in their quantum wells.
Another explanation about the scheme of the quantum well is the probability zones that oxidation o reduction of one substance occurs with another.

There are three probable zones. The area most likely to occur an interaction is below the red dotted line. The average probability zone is located between the two dotted lines. The zone of least probability is located above the blue line.

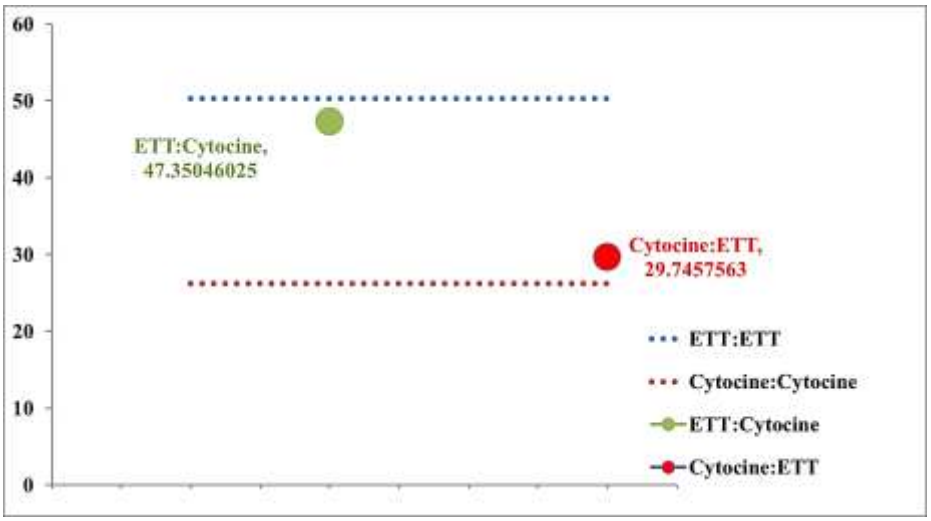

Figure 2. Quantum well. The red dot represents the Cytosine-ETT interaction. This red dot is at the bottom of the quantum well.

In general, the six quantum wells are located in the medium probability zone. Those six wells have the lowest ETCs (table 4).

CONCLUSION

In the first block we find:

1. Water has the highest ETC value of all. Water can attack or combine with all nitrogenous bases.
2. The second largest value is the ETC of the ETT. Therefore, the ETT can also attack or combine with any nitrogenous base. However, this makes it dangerous because it is no water.

In the second block we find:

1. The lowest values of ETCs were presented om the six interactions (10 to 15, table 4).
2. In these six interactions, the ETT carries the role of the oxidizing agent.
3. All these values of the six interactions fall in the zone of average probability.

It is in general concluded that:
ETT is an oxidizing agent of the nitrogenous bases of both DNA and RNA, and due to its average probability, the damage it can cause is slow. It is not fulminating.

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