

Topology on Nature: Isomerization of Five Membered Ring Tetrahedral Angles

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Abstract: Tetrahedral angles of five membered ring are disclosed from the polyhedron geometry point of view, dodecahedron and icosahedron geometry under Fibonacci number. The number of carbons on carbasugar follows the Fibonacci sequence, each carbon is placed at 0.618034 per turn (222.5[deg]). The Fibonacci golden angle 137.5[deg] with its 0.382 turns is approximately equals with Sunflower (Ferment's spiral – golden angle 136.18[deg]), icosahedron (138.16[deg]), or icositetrahedron (136.18[deg]). In case of five membered ring iminocyclitols are established four equations 18-21 for calculation the isomers of tetrahedral angles φ_{C_n} [deg] under Fibonacci approach. As demonstrate by Aston et al in 1941 and confirmed by Pitzer in 1945, the cyclopentene conformation is puckered and the deformation is not static is dynamic, with the puckering displacements progressing pseudorotation. In case of five membered ring iminocyclitols with α -D ribitol (1-5) and β -L ribitol (6-8) stereochemistry the wave character of the NMR data on 3-sphere approach – Hopf fibration *versus* Lie algebra – point out the existence of the pseudorotation through the values of tetrahedral angles φ_{C_n} [deg] around the five membered ring in close relationships with dihedral angles $\theta_{H_nH_{n+1}}$ [deg] and vicinal angles ϕ [deg], angles result from vicinal coupling constant $^3J_{H_nH_{n+1}}$ [Hz]. Hückel theories under Hopf fibration and polyhedron geometry confirming the existence of tetrahedral angles able to fluctuate around the ring. The Fibonacci approach highlighting the existence of the pseudorotation through three characteristics number: 1.6, 1.9, 1.5 calculated from carbon chemical shift δ_{C_n} [ppm] with equations 18-21. The main question, is that only a problem of geometry? or with some exception three indubitable isomers must be considered responsible for puckered five membered ring structure on its pseudo rotational itinerary. If you are exciting about this question follow the demonstration about the implication of topology on nature.

Keywords: Tetrahedral Angle, Isomerization, Pseudorotation, Fibonacci Number, Golden Ratio, Golden Triangle, Polyhedron Geometry, 3-Sphere

1. Introduction

The genetic material DNA and RNA of a virus is enclosed in capsid with either helical or icosahedral geometry. Some examples of viruses with icosahedral structure: Hepatitis C, west Nile, both class of flaviridae family, group: IV ((+) ssRN. The DNA molecule measures 34 [A⁰] long and 21[A⁰] wide for each full cycle of its double helix spiral, both number of Fibonacci series, with their ratio 1.6190476 closely approximates Phi (1.6180339). As five petals on the buttercups, the number of carbons on carbasugar follows the Fibonacci sequence, each carbon is placed at 0.618034 per

turn (222.5[deg]). The Fibonacci golden angle 137.5[deg] with its 0.382 turns is approximately equals with Sunflower (Ferment's spiral – golden angle 136.18[deg]), icosahedron (138.16[deg]), or icositetrahedron (136.18[deg]). [1]

The antiviral activity of five membered ring carbasugar or iminosugar has been demonstrated to date. [2] Platonic solid: dodecahedron (116.56[deg]) dual of icosahedron, or Catalan solid: pentagonal isositetrahedron dual of snub cube (138.18[deg]), are representative polyhedron of five membered ring and six membered ring. [3]

The first two numbers in the Fibonacci sequences are 1 and 1, or 0 and 1, and each subsequent number is the sum of the previous two. Same as Fibonacci sequences is the Lucas numbers,

in this case start with 2 and 1, all paced at 0.618034 per turns. Pascal's triangle characteristics for NMR data occurs in the sums of shallow diagrams from the Fibonacci numbers. [1]

The sequence F_n of Fibonacci numbers is defined by the recurrence relation:

$$F^n = F^{n-1} + F^{n-2}, \quad (1)$$

with: $F_1 = 1, F_2 = 1, F_0 = 0, F_1 = 1$.

$$F^n = \frac{\varphi^n - \psi^n}{\varphi - \psi} = \frac{\varphi^n - \psi^n}{\sqrt{5}} \quad (2)$$

Golden ratio:

$$\varphi = 1 + \frac{\sqrt{5}}{2} = 1.6180339887 \quad (3)$$

$$\psi = 1 - \frac{\sqrt{5}}{2} = 1 - \varphi = -1/\varphi \sim -0.6180339887 \quad (4)$$

$$\psi = -\varphi^{-1} \quad (5)$$

$$F_n = \frac{\varphi^n - \psi^n}{\sqrt{5}} = \frac{\varphi^n - (-\varphi)^{-n}}{2\varphi - 1} \quad (6)$$

Since φ, ψ are both solutions of the equations:

$$\varphi^n = \varphi^{n-1} + \varphi^{n-2}, \quad (7)$$

$$\psi^n = \psi^{n-1} + \psi^{n-2}. \quad (8)$$

In case of regular pentagon, with its golden rectangle, for any values a and b:

$$U_n = ax\varphi^n + bx\psi^n, \quad (9)$$

with $\frac{a+b}{a} = \frac{a}{b} = \varphi$.

The rhombic triacontahedron, a convex polytope where all faces are golden rhombic with the highest diagonal equal with φ , have the dihedral angles between two adjacent rhombic 144[deg], twice the isosceles angles of a golden triangle, and four times its acute angle. The silver ratio of Pell number is $1 + (2)^{1/2}$, the parallel side of trapezoid to other side equal with 1, geometry found in 5 and 7 membered ring. [3]

Polyhedrons dodecahedron dual of icosahedron:

$$\tan \frac{D^U}{2} = A = 2 \sin \frac{X}{2} \quad (10)$$

$$\tan \frac{D^I}{2} = A^2 = 2 \sin \frac{X}{2} \quad (11)$$

with D^U and D^I dihedral angles of dodecahedron and icosahedron.

Rhombic polyhedron geometries, rhombic dodecahedron with acute and obtuse angles drawn inside of the sphere [3]:

$$\text{Acute angle: } \alpha = 2 \tan^{-1} \frac{1}{1.618034} \quad (12)$$

$$\text{Obtuse angle: } \beta = 2 \tan^{-1} 1.618034 \quad (13)$$

Golden triangle [3]: $\varphi^G = 1.6180339887$.

$$\frac{Y}{2} = \cos^{-1} \frac{\varphi^G}{2} = \frac{\pi}{5} = 36^{\text{deg}} \quad (14)$$

$$\varphi_{C_n} = 180 - \gamma = 108^{\text{deg}} \quad (15)$$

$$2 \times \cos^{-1} \frac{1}{\varphi^G} = 103.6545^{\text{deg}} \quad (16)$$

$$\tan \frac{103.65}{2} = 2 \times \sin^{-1} \frac{1.27191}{2} = 78.98, 101.017 \quad (17)$$

where: γ – internal angle[deg], φ_{C_n} – tetrahedral angle[deg].

2. Calculation of the Isomers of Tetrahedral Angles and Corresponding Polyhedron Values

2.1. Method for Calculation of the Isomers of Polyhedron Values

Tetrahedral angles of five membered ring can be calculated from chemical shift using the polyhedron characteristics numbers 1.6 – dodecahedron and 2.4 – icosahedron. [4, 5] In attempt to demonstrated the existence of three representative values (1.61, 1.9, 1.5) between isomers of five membered ring tetrahedral angles φ_{C_n} [deg], are developed the equations 18 and 19 for calculation Y from X and Z from Y, since with equations 20 and 21 can be calculated X from Y and Z from Y (Table 1).

$$\frac{16}{(X^n)^2} = Y, \quad (18)$$

Where: $n = 2: C_1, C_4; n = 1: C_2, C_3$

$$\frac{X^2}{2} = \frac{2}{\sqrt{Y}} \quad (19)$$

$$Y^{1/4} = W; 2 \times W = Z^2 \quad (20)$$

$$Z^2 = 2 \times W; W^4 = Y \quad (21)$$

2.2. Calculation of the Isomers of Tetrahedron Angles

The isomers of tetrahedral angles can be calculated from tetrahedral values with eq. 22, 23: step 1. from the energy calculated from carbon chemical shift are calculated first the polyhedron number X 1.6, Y 1.9, Z 1.5, step 2: with eq. 22 are calculated tetrahedral, internal or polyhedron angle, step 3: with eq. 23 are transformed polyhedron angles in tetrahedral angles. In table 1 are presented the calculated polyhedron numbers with eq. 18-21 for iminocyclitols with α -D ribitol (1-5) and β -L ribitol (6-8) stereochemistry. [6, 7]

$$\theta_1 \text{ or } \theta_2 = (1/P) \times 180[\text{deg}] \quad (22)$$

$$\tan \frac{\theta_1}{2} = P' = 2 \times \sin \frac{\theta_2}{2} \quad (23)$$

Where: $P = X, Y, X$ result from eq. 18-21 and numerated with 1, 2, 3 in table 1; θ_1 or θ_2 : φ – tetrahedral angle or γ – internal angle, $\varphi + \gamma = 180[\text{deg}]$, P' other polyhedron values; *i.e.* $\tan^{-1} 1.618029 = 116.564[\text{deg}]$, $\sin^{-1} 1.618029 = 107.999[\text{deg}]$, $\tan^{-1} (1.618029)^2 = 138.189[\text{deg}]$, $\sin^{-1} (1.618029)^2 = 99.264[\text{deg}]$, $2 \times \tan^{-1} \{2 \times \sin[(180 - 99.264)/2]\} = 104.66[\text{deg}]$, $2 \times \tan^{-1} \{2 \times \sin[(180 - 104.459)/2]\} =$

101.548[deg].

Table 1. Calculation of the polyhedron representative numbers (X, Y, Z [J/moli $\times 10^6$]) of iminocyclitols 1-8 with eq. 18-21 and the corresponding tetrahedral angles calculated with eq. 22, 23.

Entry	C_n [ppm] φ_{C_n} [deg]	$^3J_{HnHn+1}$ [Hz]	1 E[J/moli $\times 10^6$]	2	3	Entry	C_n [ppm] φ_{C_n} [deg]	$^3J_{HnHn+1}$ [Hz]	1 E[J/moli $\times 10^6$]	2	3
1.	1-C ₁ : 56.6	-	1.69415	1.94225	1.53657	41.	5-C ₁ : 3.7	4.8	1.90667	1.70200	1.53302
2.	φ_{C1} [deg]		106.247	108.174 106.764 ^e	103.762	42.			107.298	107.775	103.409
3.	1-C ₂ : 82.7	-	2.47538 ^d 1.57333 2.34666 ^d 1.53188	1.89531	1.70454 1.61591	43.	5-C ₂ : 72.5	5.2	2.17007	1.647825	1.55802
4.	φ_{C2} [deg]		101.781 103.295 2.51130 ^d 1.58470 2.48585 ^d 1.57666 2.38662 ^d 1.54487 101.543	107.0	107.344 ^e	44.	φ_{Cn} [deg]		107.794 100.626	109.234 108.601	107.659
5.	1-C ₃ : 83.9	-	1.184154 1.5389313 103.996 109.245	2.02777	1.67600 1.60910	45.	5-C ₃ : 4.0	5.2	2.214974	1.639410	1.56201
6.	φ_{C3} [deg]		101.134 101.472	108.882	107.379 109.796	46.	φ_{Cn} [deg]		107.794 101.226	109.234 106.924	107.659
7.	1-C ₄ : 66.1	-	1.97851	1.686340	1.540129	47.	5-C ₄ : 9.3	0	2.074294	1.666527	1.5492581
8.	φ_{C4} [deg]		108.525	106.739	101.765	48.	φ_{Cn} [deg]		107.900 106.285 ⁱ	107.521	101.200
9.	1-NH: 5.29	-	0.844484 1.184154 1.5389313 103.996 109.245	1.96622	1.68896	49.	5-NH: -	-	-	-	-
10.	φ_{NH} [deg]		107.77 2.49932 1.58092 2.43878 1.56166 100.32 101.743 2.52327 1.58848 2.53360 1.59172 2.57534 1.60478	108.730	106.573	50.	φ_{Cn} [deg]		2.047355 107.447	1.671982 107.656	1.5080611 101.357
11.	2-C ₁ : 55.8	4.1	1.670210	2.05605	1.54754	51.	6-C ₁ : 8.4	4.8	2.047355	1.671982	1.5080611
12.	φ_{C1} [deg]		107.77 2.49932 1.58092 2.43878 1.56166 100.32 101.743 2.52327 1.58848 2.53360 1.59172 2.57534 1.60478	107.073	101.306	52.	φ_{Cn} [deg]		107.447	107.656	101.357
13.	2-C ₂ : 83.5	5.3	1.670210 107.77 2.49932 1.58092 2.43878 1.56166 100.32 101.743 2.52327 1.58848 2.53360 1.59172 2.57534 1.60478	2.21094	1.64015	53.	6-C ₂ : 1.1	5.2	2.128171	1.655877	1.5542319
14.	φ_{C2} [deg]		101.078 101.083	106.131	109.745	54.			106.769	107.186	100.728
15.	2-C ₃ : 84.3	5.3	1.972524 1.68761 1.53954 1.5389313 103.996 109.245	2.11680	1.60478 1.65809	55.	6-C ₃ : 2.7	5.2	2.176063	1.646691	1.5585614
16.	φ_{C3} [deg]		101.078 101.083	107.007	106.423 108.558	56.			107.447	106.893	101.329
17.	2-C ₄ : 65.9	0	1.972524 1.68761 1.53954 1.5389313 103.996 109.245	1.68761	1.53954	57.	6-C ₄ : 0.9	0	2.122185	1.657044	1.5063703
18.	φ_{C4} [deg]		108.249 0.421443 2.372795 1.540387 101.749 108.896	106.659	101.801	58.			106.895	107.223	100.650
19.	2-NH: 2.64	-	1.718102 1.836217 1.525827	1.68577	1.98116	59.	6-NH:-	-	-	-	-
20.	φ_{NH} [deg]		106.638 ^f 106.256	106.775	108.646	60.			1.8947015 106.989	1.7046875 107.752	1.531819 103.289
21.	3-C ₁ : 57.4	3.1	1.718102 1.836217 1.525827	1.836217	1.525827	61.	7-C ₁ : 3.3	2.8	1.8947015	1.7046875	1.531819
22.	φ_{C1} [deg]		106.638 ^f 106.256	106.771	102.685	62.			106.989	107.752	103.289
23.	3-C ₂ : 71.5	3.9	2.140144 1.653557 1.555322	1.653557	1.555322	63.	7-C ₂ : 2.1	3.6	2.1581039	1.6501062	1.5569477
24.	φ_{C2} [deg]		106.519 108.856 101.502 ^g	100.825		64.			106.145	107.002	101.108
25.	3-C ₃ : 71.7	3.9	2.140144 1.653557 1.555322	1.652402	1.555865	65.	7-C ₃ : 3.4	3.6	2.1970156	1.6427508	1.5604294
26.	φ_{C3n} [deg]		106.394 108.932 100.897 ^g	100.791		66.			107.717	106.766	101.580
27.	3-C ₄ : 66.8	8.8	1.999463 1.681905	1.681905	1.542159	67.	7-C ₄ : 3.9	8.8	1.9126607	1.7006717	1.5336269
28.	φ_{C4} [deg]		109.448 107.021 101.640	107.021	101.640	68.			107.450	107.786	103.469
29.	3-NH: 3.33	-	0.531593 1.707728	1.707728	1.530444	69.	7-NH: -	-	-	-	-

Entry	C _n [ppm] φ _{C_n} [deg]	³ J _{HnHn+1} [Hz]	1 E[J/moli×10 ⁶]	2	3	Entry	C _n [ppm] φ _{C_n} [deg]	³ J _{HnHn+1} [Hz]	1 E[J/moli×10 ⁶]	2	3
30.	φ _{NH} [deg]	-	1.881134			70.	-	-	-	-	-
31.	4-C ₁ : 57.8	-	1.730075	1.785912 ^d 1.875541	1.520538	71.	8-C ₁ : 77.9	-	2.3317100 1.5269938	1.847473	1.71.5479
32.	φ _{C₁} [deg]	-	107.716 ^h	100.78 106.47	102.146	72.			102.803	107.73	107.660
33.	4-C ₂ : 71.9	-	2.152117	1.651252	1.556407	73.	8-C ₂ : 5.0	3.9	2.2449070	1.6339185	1.5989047
34.	φ _{C₂} [deg]	-	106.269	106.8001	101.033	74.			107.579	106.478	100.634
35.	4-C ₃ : 74.1	-	2.217968	1.638857	1.562281	75.	8-C ₃ : 8.8	3.9	2.0593280	1.6695468	1.5478564
36.	φ _{C₃} [deg]	-	107.657	107.723	101.824	76.			106.932	107.813	101.287
37.	4-C ₄ : 69.4	-	2.077287	1.665926	1.549537	77.	8-C ₄ : 4.9	9.1	2.2419138	1.6344636	1.5643803
38.	φ _{C₄} [deg]	-	107.837	108.047	100.028	78.			107.587	106.496	103.584
39.	4-NH: 2.2	-	2.847354 1.687410	1.973501	1.539641	79.	8-NH: -	-	-	-	-
40.	φ _{NH} [deg]	-	106.672	108.295	101.795	80.					

a. δ_c, δ_H[ppm], ¹H 400MHz, ¹³C 75MHz: 1-CDCl₃, 2-CDCl₃, 3-D₂O, 4-CDCl₃, δ_H 5-CDCl₃, δ_c 6-CD₃OD, δ_H 7-CD₃OD, δ_H 8- CD₃OD; b. E = δ_{C_n}×ω_C×h×N_A[J/moli×10⁶]; h - 6.626176×10⁻³⁴ [Jxs], N_A - 6.023×10²³ [moli⁻¹], n = 1, 1/2, 2, c. 1/(R_m^B)², φ_{C₁}: sin84.56/2 = 2×tan2A; d. eq. IB (Entry 3): 1.7857: 100.79, 101.41[deg], 1.7977: 100.12, 100.66; eq. IB (Entry 5): 1.78255: 100.98, 101.63[deg], 1.7848: 100.85, 101.49[deg], 1.793: 100.33, 100.90[deg]; e. tan{[1/(1.7045)^{1/2}]×180}/2 = 2xsin⁻¹(2.5962)^{1/2} = 107.344 = tan{1/(1.6159)²}×180×2/2; f. 1/E: 101.35, 1/E²: 106.63, 1/E^{1/2}: 106.25; g. 1/E²: 101.14; h. 1/E^{1/2}: 105.332, 115.673 under polyhedron unit 107.716[deg]; 1/E²: 119.86, 119.45, 117.87, 112.20, 106.37[deg]; i. 1/E: 107.90, 1/E²: 106.28.

As observation in case of five membered ring, the following values are representative for C₁ and C₄: 1.6 and 1.9 and for C₂ and C₃: 2.4 – 2.5; ~ 1.79 resulting in case of 1-C₂ and 1-C₃ from three and two transformations with eq. 21 (Table 1, entry 3 and 5) increasing the tetrahedral angles with values ~100[deg]. In

case of 4-C₁ are calculated the following values 1.73007, 1.7859 and 1.52053 with tetrahedral angles 107.71, 100.78, and 102.146. Using the eq. 21 after two transformations from 1.7859 result Y = 1.87554, with the corresponding tetrahedral angle of 106.47[deg] (Table 1, entry 31, 32).

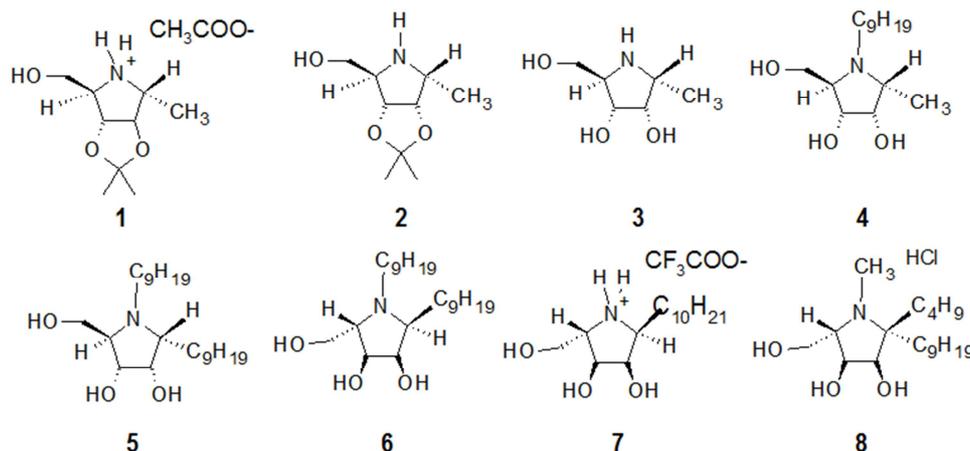


Figure 1. Iminocyclitols with α-D ribitol (1-5) and β-L ribitol (6-8) stereochemistry.

The nature of the substituents, isopropylidene group 1, 2, alkyl chain at nitrogen 4, 5, or acetate salt 1, introduces some change. Isopropylidene iminocyclitols 3 and 4 have at C₁ a borderline value between X = 1.6 and Y = 1.9, respectively 1.7 for C₁ and 2.0 - 2.2 for C₂ and C₃. Iminocyclitols 5 and 6 bearing nonyl chain at nitrogen and C₁, and trifluoroacetate salt 7 bearing decyl chain at C₁ have all first calculate values from carbon chemical shift equals with Y = 1.9 – 2.2. Polyhedron numbers of the iminocyclitols 6, 7 with higher antiviral activity are at borderline between dodecahedron and icosahedron values. Iminocyclitol 8 bearing butyl and nonyl at C₁ and methyl at nitrogen, also with higher biological activity, has 8-C₁ under Z rule (21) and 8-C₂₋₄ under Y rule (19). Applying eq. 18, 19 and 20, 21, result three values from only one carbon chemical shift which highlighted the interval of

change in function of substituents: a. in case of C₁ and C₄ two values 1.6 and 1.9 are characteristics, with tetrahedral angles sometimes almost equals probably as consequence of the trigonometry around of molecules, and the third value (~1.53), the square values of 2.36 with tetrahedral angles characteristics for C₂, C₃; b. in case of C₂, C₃ two values are characteristic, respectively 2.4 or 2.1 along 1.6 calculated usually for C₁, C₄.

Icosahedral geometry having the minimum of defects relative to spherical coordinate, can explain the values of tetrahedral angles at NH, since the total value of the tetrahedral angles sum in pentagon is 540[deg]. The reported tetrahedral angles of five membered ring cyclic amine are φ_{NH} 108.0, φ_{C₁} 108.1, φ_{C₂} 107.6[deg], with I_{NHC1} 1.383[A⁰], I_{C1C2} 1.371[A⁰], I_{C2C3} 1.429[A⁰], and of five membered ring cyclic

ether are φ_{NH} 106.0, φ_{C1} 110.9, φ_{C2} 106.1[deg], with l_{NHCl} 1.37[Å], l_{C1C2} 1.35[Å], l_{C2C3} 1.44[Å]. [8] Methyl β -D-ribofuranoside with ${}^2E - {}^1T_2$ conformation (P -25.99[deg]) has as resulted from X-ray the following dihedral angles φ_{C1} 106.4, φ_{C2} 100.8, φ_{C3} 103.9[deg], φ_{C4} 109.1[deg] relative to φ_{C4} 110.2[deg] as result from neutron diffraction crystal structures. [9]

The length $l_{CC}[A^0]$ can be calculated from half internal angle with eq. 24, internal and tetrahedral angles are under torus eq. 25.

$$l_{CnCn+1} = 2 \times \cos \frac{\gamma}{2} \quad (24)$$

where: l_{CnCn+1} – length between two tomes of carbon [Å]
 γ – internal angle[deg]

$$\sin \frac{\varphi}{2} \cos X = \frac{\gamma}{2} \quad (25)$$

where: φ – tetrahedral angle[deg], $180 - \gamma = \varphi$.

2.3. Energy and Euclit Golden Ratio Under 3-Sphere and Polyhedron Approach

Tetrahedral angles [10] are calculated from carbon chemical shift in opposite – sphere/invers of sphere – sin/tan functions- with dihedral angles [11-13] of five membered ring: step 1 are calculated the invers of polyhedron values, step 2 are calculated angles X and Y with trigonometric eq. 26, 27 from $E^n[J/moli \times 10^6]$ with $n = 1, \frac{1}{2}, 2$, step. 3. are established the relationship between tetrahedral and dihedral angles in opposite. [14]

$$\tan^{-1} \frac{1}{E^n} = X \quad (26)$$

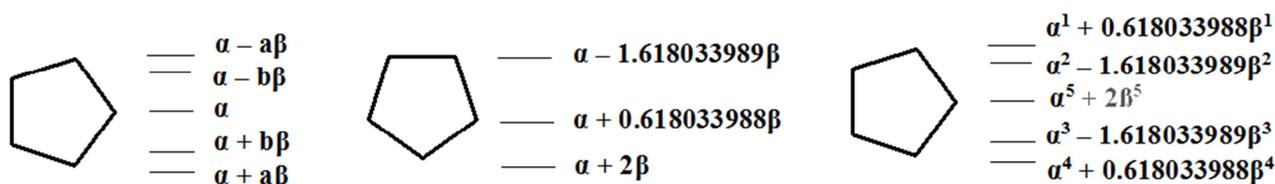


Figure 2. Five membered ring on Hückel theory and golden ratio.

2.5. Polyhedron Equation on Isomerization of Internal and Tetrahedral Angles of Five Membered Ring

Table 2. Tetrahedral angle φ_{C1} [deg] of iminocyclitol 2 calculated from carbon chemical shift with polyhedron unit.

Entry	1/E	1/E ^{1/2}	1/E ²		
1.	63.95		62.49		
	73.55	78.61	68.99	73.52	62.48
	75.91	77.80	74.14	79.75	71.54
	79.73	76.56	82.87	84.02	87.89
	100.26	101.38	97.12	95.97	92.10
	104.08	102.19	105.85	100.24	108.45
	106.44	103.42	111.00	106.47	117.51
	116.05		117.51		
2.	2-H ₁ H ₂ : ³ J _{H₁H₂} [Hz] 4.15; Φ [deg] 68.99				
	θ_{HnHn+1} [deg] 21.00; φ_{C1} [deg] 106.47, 108.45				

In table 2 are presented internal and tetrahedral angles

$$\sin^{-1} \frac{1}{E^n} = Y \quad (27)$$

Where: $E = \delta_{Cn} \times \omega_C \times h \times N_A [J/moli \times 10^6]$: δ_{Cn} [ppm], ω_L : ¹³C 400[MHz], $h - 6.626176 \times 10^{-34} [Jxs]$, $N_A - 6.023 \times 10^{23} [moli^{-1}]$, $n = 1, \frac{1}{2}, 2$, φ – tetrahedral angle or γ – internal angle = $2 \times X$ or $2 \times Y$, $\varphi + \gamma = 180$ [deg], ϕ – vicinal angle[deg], $\phi = (n \times {}^3J_{HH})^2$, *trans-aa* $n = 1$, *cis, trans-ee* $n = 2$.

2.4. Euler-Hückel I-Polyhedron Approach

Tetrahedral angles can be calculated with Huckel I (Figure 2, eq. 28, 29) from carbon chemical shift δ_{Cn} [ppm] under sin/cos or tan function, Euler tessellation of the geodesic triangles (eq. 30-32). Polyhedron angles are transformed in tetrahedral angles with polyhedron eq. 10, 11. [15]

Hückel I:

$$E = \alpha + 2m_i \times \beta \quad (28)$$

$$B = 2m_i \times \beta = (E - \alpha) \quad (29)$$

Euler tessellation:

$$C_1, C_4 \varphi = 2\sin^{-1}B, C_2, C_3 \varphi = 2\cos^{-1}B \quad (30)$$

$$C_1, C_4 \gamma = 2\tan^{-1}B, C_2, C_3 \theta^D = 2\tan^{-1}B \quad (31)$$

$$\gamma \text{ or } \theta^D = 90 \times B \quad (32)$$

Where: $m_i = \cos(2\pi j^3/n^3)$

Angular momentum: $j^3 = 1 - 7$

Quaterionic: $m_i = i, j, k, -i, -j, -k$

φ – tetrahedral angle[deg], γ – internal angle[deg], θ^D – polyhedron[deg]

calculated from carbon chemical shift φ_{C1} [deg] for iminocyclitol 2 using polyhedron eq. 10, 11. The relationship between tetrahedral angles and dihedral angles was demonstrated with *polyhedron unit*, six angles - three internal and three tetrahedral, the number of angles increasing until the vicinal coupling constant can be calculated from the relationship vicinal angle ϕ [deg] - the dihedral angle θ_{HnHn+1} [deg].

For a vicinal coupling constant of 4.1[Hz] result an angle of 111[deg]. unexpected for a tetrahedral angle of five membered ring, but is in relationship of 180 with the vicinal angle. At this stage the polyhedron rule is in contradiction with the square of energy rule ($1/E^2$), the dodecahedron value of E (1.670 J/moli $\times 10^6$) giving an angle of 106.442[deg] for set A ($1/E$) *Considering all isomers*: from the square of energy result an angle of 106.478[deg] almost equal with angle calculated

from set A (1/E), and from an angle of 95.971[deg] under the polyhedron unit result an angle of 106.478[deg] almost equal with angle calculated from 1/E. [10, 14]

Table 3. Isomerization of the tetrahedral angles with polyhedral approach.

Entry	I.	II.	III.	IV.
1.	61.18	64.48	75.11	66.70
	71.00	72.35	78.72	73.23
	88.99	86.28	81.12	84.57
	91.00	93.71	98.87	95.42
	108.99	107.65	101.27	106.76
	118.82	115.51	104.88	113.29

An alternative method for calculation tetrahedral angles using polyhedron eq. 10 and polyhedron unit of 6 angles is presented in table 3.

From the six's angle of first set (I) is calculated the six's angle of second set (II), then the six's angle of third set (III). The six's angle of forth (IV) result from the angle 98.87[deg] of set (III). [5]

3. Results and Discussion

As presented in table 1, from carbon chemical shift transformed from ppm in $J/\text{moli} \times 10^6$ are calculated all possible isomers with eq. 18, 19 and 20, 21, then the corresponding tetrahedral angles with Fibonacci golden angle and polyhedral eq. 22, 23. For all atoms of carbon are calculated two angles $\sim 106 - 109$ [deg] and one angle $\sim 100 - 103$ [deg]. At this stage the main question was that is it possible to have values around 100[deg] at C_1 and C_4 and values around 106[deg] at C_2 and C_3 ?

Table 4. Tetrahedral angles calculated in close relationships with dihedrals and vicinal angles with 3-sphere approach.

Entry	Comp.	Comp. 2			
1.	C_n [ppm]	C_1 55.8	C_2 83.5	C_3 84.3	C_4 65.9
2.	$E[J/\text{moli} \times 10^6]$	1.67215	2.49932	2.52322	1.97252
3.	$^3J_{\text{HnHn+1}}$ [Hz]	4.1	5.3	5.3	0
4.	$1/E^{1/n}$	$1/E^2$	$1/E^2$	$1/E^{1/2}$	$1/E^{1/2}$
5.	sin or cos	ϕ 69.044			θ_{H3H4} 90.798
		$^3J_{\text{H1H2}}$ 4.81			$^3J_{\text{H3H4}}$ 0.446
		θ_{H1H2} 20.95	ϕ_{C_2} 101.524	ϕ_{C_2} 101.968	ϕ_{C_4} 101.349
6.	tan	ϕ_{C_1} 100.477 ^a			ϕ_{C_4} 101.134 ^b
		ϕ_{C_1} 100.664 ^b	ϕ 115.369	ϕ 115.616	
			$^3J_{\text{H2H3}}$ 5.57	$^3J_{\text{H2H3}}$ 5.37	
6.	tan		θ_{H2H3} -25.36	θ_{H2H3} -25.61	
			ϕ_{C_2} 106.157 ^c	ϕ_{C_3} 106.095 ^c	ϕ_{C_4} 109.097
			ϕ_{C_2} 107.594 ^b	ϕ_{C_3} 107.693 ^b	

Entry	Comp.	Comp. 3			
1.	C_n [ppm]	C_1 63.7	C_2 72.5	C_3 74.0	C_4 69.3
2.	$E[J/\text{moli} \times 10^6]$	1.90667	2.17607	2.21497	2.07429
3.	$^3J_{\text{HnHn+1}}$ [Hz]	4.8	5.2	5.2	0
4.	$1/E^{1/n}$	$1/E^{1/2}$	$1/E^{1/2}$	$1/E^{1/2}$	$1/E^{1/2}$
5.	sin or cos	ϕ 92.805	94.495	95.569	θ_{H3H4} 92.0525
		$^3J_{\text{H1H2}}$ 4.81	ϕ_{C_2} 101.118	ϕ_{C_3} 100.553	$^3J_{\text{H3H4}}$ 0.716
		θ_{H1H2} -2.8			
6.	tan	ϕ_{C_1} 101.6006 ^a			ϕ_{C_4} 101.5065 ^a
		ϕ_{C_1} 101.3773 ^b	ϕ 111.660	ϕ 112.204	ϕ_{C_4} 101.792 ^b
			$^3J_{\text{H2H3}}$ 5.283	$^3J_{\text{H2H3}}$ 5.296	
6.	tan		$\theta_{\text{HnHn+1}}$ -21.66	$\theta_{\text{HnHn+1}}$ -22.204	69.5466
			ϕ_{C_2} 107.084 ^c	ϕ_{C_3} 106.948 ^c	ϕ_{C_4} 107.386
			ϕ_{C_2} 106.116 ^b	ϕ_{C_3} 106.331 ^b	

a. $[(\phi/4)/2] + 90$; b. polyhedron unit: $\phi_{C_n} = 2 \times \tan X = 2 \sin \theta^3/2$, $\theta^3 = 180 - \phi$; c. $[(180 - \phi)/2] + 90$

Tetrahedral angles calculated from carbon chemical shift δ_{C_n} [ppm] in opposite, *i.e.* dihedral $\theta_{\text{HnHn+1}}$ [deg] and vicinal ϕ [deg] angles from sin function and tetrahedral ϕ_{C_n} [deg] from tan function or *vice versa* (Table 4), a Torus - Dupin cyclide approach, [14] shown that the angles calculated from tan function for C_1 and C_4 are two higher ($1/E^2$ 109[deg] characteristic for six membered ring, $1/E$ 106.541[deg] over rule, is not in close relationship with vicinal angle, but can be transformed under polyhedron unit rule, table 2: $\sin^{-1} 1/E^2 = 20.9555$ [deg], a. $90 + 20.955 = 110.955$ [deg] = ϕ , b. 20.955×4

= 83.822, 106.368[deg]), in opposite with angles characteristics for 2- C_2 100.6 and 2- C_3 101.3[deg] result from sin function. Angles calculated for 2- C_2 101.5 and 2- C_3 101.9[deg] from sin function are in opposite with are angles characteristics for 2- C_1 106.1 and 2- C_4 106.0[deg], calculated from tan function. Dihedral angle $\theta_{\text{HnHn+1}}$ [deg] and corresponding vicinal coupling constant $^3J_{\text{HnHn+1}}$ [Hz] results from sin function in case of 2- C_1 and 2- C_4 and from tan function in case of 2- C_2 and 2- C_3 , under 3-sphere approach. Thus, iminocyclitols 2 have C_1 under $1/E^2$ rule and C_2 , C_3 , C_4

under $1/E^{1/2}$ rule, with values of C_1 and C_4 around 109[deg]: 109.67^T, 101.52^S, 101.96^S, 109.09^T, isomers: 100.47^S, 106.15^T, 106.09^T, 101.34^S, polyhedron unit: 100.66, 107.59, 107.69, 101.349. Iminocyclitols 5 have the calculated tetrahedral angles 108.17^T, 101.118^S, 100.55^S, 107.38^T[deg] with the following isomers result from the opposite trigonometric function 101.6^S, 107.08^T, 106.94^T, 101.506^S[deg], all angles resulting from $1/E^{1/2}$. The isomers angles calculated with polyhedron unit are: 101.377, 106.116, 106.331, 101.554[deg]. If the calculated angles for C_1 and C_4 are subject to polyhedron unit probably the values of tetrahedral angles are decreased. In table 2 is presented a method for building unit from internal and polyhedron unit, resulting for $1/E^2$ two possible tetrahedral angles 106.47, 108.45. Under 3-sphere unit [13] was state that two pairs of angles 106, 103[deg] on tan unit and

108, 101[deg] on sin unit are in close relationship with dihedral angles: θ_{H1H2} 22.84[deg] for a vicinal coupling constant of 4.1[Hz] and a tetrahedral angle φ_{C1} 106[deg], and θ_{H2H3} -27.61[deg] for a calculated vicinal coupling constant of 5.4[Hz] and a tetrahedral angle φ_{C2} of 101[deg]. [14]

A switch between the vicinal coupling constant and tetrahedral angles are shown in table 4 relative to angles calculated in opposite from sin and tan function? Can be considered tables 1 and 4 under pseudorotation motion?

The deviation from planarity of five membered ring can be represented as graph vertex in the spherical coordinate or as platonic solids with Euclidean pentagons or triangles. In plan Euler's polygon division gives a pentagon governed by the golden ratio, and Fibonacci numbers.

Table 5. Tetrahedral angle φ_{Cn} [deg] of iminocyclitol 3 calculated from carbon chemical shift with Euler -Hückel I.

Entry	φ_{C1}	φ_{C2}	φ_{C3}	φ_{C4}	φ_{C5}
1. ^a	106.26	102.63	-102.63	-106.25	N 4:-104.47, -112.29 N -1.6: 102.63, 111.45 N 1.6: -102.63, -111.66 N 4: -112.28
2. ^b	102.68	115.98	-115.98	-102.31	N -1.6: 115.98, N 1.6: -115.98 N 4:-106.26, -112.29 N -1.6: 106.26, 112.29 N 1.6: -106.26, -112.29
3. ^c	102.68	106.26	-106.74	-102.31	

a. Cos/sin-Euler- Hückel I, b. Tan-Euler- Hückel I, c. Tan-Euler- Hückel I Dodecahedron.

Euler -Hückel I tetrahedral angles calculated with eq. 28, 29 under sin/cos (eq. 30) or tan trigonometric (eq. 31) function for iminocyclitol 3 shown same alternation of the tetrahedral angles around the five membered ring (Table 5). 3-sphere in 4D involve quaternions multiplications (H). A collection of fibers over circles in S^2 is a torus ($S^1 \times S^1$), with cylindrical coordinates, a limit case of the conic.

Bloch sphere is a geometrical representation of the pure

state space of two-level quantum mechanical system (Qubit), mapped as Riemann sphere, in two-dimensional Hilbert space is the complex projective line CP^1 , 2-sphere unit known as Poincare sphere. Mapped as 3-sphere unit, two-dimensional state space C^2 , known as Hopf fibration. Hückel theory on 3-sphere, spherical representation on higher dimension space with cyclic graph (Figure 3).

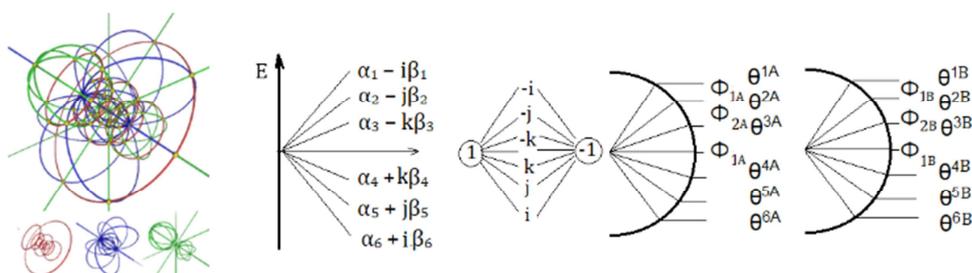


Figure 3. Spherical representation in higher dimensional space with cyclic graph.

One atom on the plane of unpuckered ring can be projected as a planar curve: $i e$. a point in Kilpatrick's model [16], an interval in the Adams model (namely AGB)[17], or an ellipse in the Herzyk-Rabczenko model [18, 19]. The HR ellipse described two characteristic directions of the unpuckered five-membered ring. Inside of 3-sphere can be found easy three sets angles, in close relationships with other four sets angles, totally seven sets angles U, S or combinations between U and S. The transformation from U to S corresponding to tan function, in other word the transformation from torus to Dupin

cyclide, and the transformation S to U corresponding to Dupin cyclide to torus transformation. [13]

Hopf fibration on 3-sphere model ensuring all relationships between Riemann sphere and corresponding cyclide resulting in multidimensional space. The vicinal coupling constant is in R^2 real fibration $S^0 \rightarrow S^1 \rightarrow S^1$ or R^4 complex Hopf fibration $S^1 \rightarrow S^3 \rightarrow S^2$. In first case is point out the direct relationship between the vicinal angle and the dihedral angle, and in second case the possibility to transform the dihedral angle in vicinal angle and the vicinal angle in dihedral angles, [13]

resulting relationships between set A and set B with two vicinal coupling constants ${}^3J_{\text{HH}}[\text{Hz}]$. All *cis/trans* stereochemistry on torus coordinates are in \mathbb{R}^{16} : octonionic Hopf fibration $S^7 \rightarrow S^{15} \rightarrow S^8$, quaternionic multiplication $S^3 \rightarrow S^7 \rightarrow S^4$, from the direct relationship between the vicinal angles and the dihedral angles. The tangential space, the transformation from torus to Dupin cyclide and *viceversa*, can be found on 14 sets angles without the corresponding sign, as demonstrated with trigonometric equations.

Circle representation of ellipse through eigenvector and eigen values enable ellipse representation on torus and Dupin cyclide of 3-sphere unit with all characteristic circles (Figure 4).

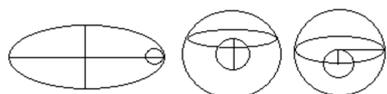


Figure 4. Ellipse representation on 3-sphere characteristic circles.

The cyclopentene conformation is puckered and the deformation is not static is dynamic, with the puckering displacements progressing pseudorotation, as demonstrate by Aston et al in 1941 thermodynamic [20] and Pitzer in 1945 based on relationship between structure and stain energy [21], confirmed by infrared spectroscopic study in 1968 [22]. The calculated tetrahedral angles along the corresponding isomers from the sin and tan function in opposite indicate a possible pseudorotation, the structures with tetrahedral angles I being the most stable. Conformational analysis of furanose ring involves the measurement of the three-bond ${}^1\text{H}-{}^1\text{H}$ coupling constant (${}^3J_{\text{HH}}$) and used one of the already published method: *i e.* PSEUDOROT [23], DAERM (“Dihedral Angles Estimation by the ratio method”) [24], molecular mechanics program [25], 3-sphere [11-13]. The PSEUDOROT program gives two conformers one in northern and other in southern hemisphere, conformers which equilibrate via pseudorotation and characterized by two coordinates Altona-Sundaralingam (AS) pseudorotational phase angle (P) and AS puckering amplitude (ϕ_m), calculated from Karplus dihedral angles. DAERM method considered the magnitude of the Karplus constants, K_1 and K_2 , vary, the ratio of K_1 and K_2 is constant. [24] The 3-Sphere approach for calculation of the dihedral angles from vicinal coupling constant under the torus – Dupin cyclide inversion gives 6 *cis/trans* dihedral angles [12, 14] from only one vicinal angle, angles restricted by the VISION molecular model on conformational/configurational analysis. [26-28] In solid state, the nucleic acid is puckered at C (2) or/and at C (3), but usually only one puckered state is observed. The puckering or pseudorotational disorder in crystals can be: I. three atoms anchored in the crystal, one endocyclic bond angle constant, restricted to one quadrant of the pseudorotational wheel, II. four atoms fixed in the crystal, one endocyclic torsion angle constant, defined by the envelope states. The mechanism between two energy minima can be via the pseudorotation in furanose ring and interconversion via the planar state in pyrrolidine rings. [29] That has been demonstrated the furanose ring bearing

substituents has hindered pseudorotation relative to cyclopentane. [30]

4. Conclusion

- Four equations (eq. 18-21) are established based on polyhedron number 1.6 and 2.5, dodecahedron *versus* icosahedron, in attempt to calculate all the isomers of tetrahedral angles of five membered ring iminocyclitols 1-8. Two values around 106-108[deg] and one around 100-103[deg] are calculate for all tetrahedral angles $\varphi_{\text{C1-4}}$ and $\varphi_{\text{NH}}[\text{deg}]$ (eq. 22, 23), having as characteristic polyhedron values 1.6, 1.9, 1.5 in table 1.
- The concept of pseudorotation was point out based on tetrahedral angles of five membered ring calculated from carbon chemical shift using Fibonacci number (1.6190476), polyhedron equation (eq. 10, 11) and units (Tables 2, 3); tetrahedral angle $\varphi_{\text{Cn}}[\text{deg}]$ result in close relationship with dihedral $\theta_{\text{HnHn+1}}[\text{deg}]$ and vicinal angles $\phi[\text{deg}]$ under 3-sphere approach – Hopf fibration *versus* Lie algebra (Table 4, eq. 26, 27), or from Hückel theories under Hopf fibration and polyhedron geometry (Table 5, eq. 28-32).

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