Graph Flux Intensity and Electromagnetic Wave on 3-sphere Approach

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Abstract: 3-Sphere characteristic angles (θ^{nN} with n = 1-6, and ϕ_{nN} with n = 1, 2, N = A, B, C, CA, CB) are calculated from NMR data, the differences in chemical shifts between two atoms of carbon $\Delta\delta_{CnCn+1}$ [ppm] and vicinal coupling constant $^3J_{HnHn+1}$ [Hz], using I. Graph-flux intensity, *Golden ratio* of pentagon, II. *radio wave,* III. *Homotopic approach*, exploring electromagnetic field of five membered iminocyclitols 1-3. Fibonacci's numbers calculated with Plank constant h and h-bar are compared and used for determination of the tetrahedral angles. Attempts to obtain the best equation for calculation the energy from carbon chemical shift: the square $E^{P2} = (\Delta\delta x\omega)^2 xhxN_A[Jx10^{-3}xrad/sxmoli]$ and the cube of frequency $E^{P3} = (\Delta\delta x\omega)^3 xhxN_A[Jxrad/s^2 xmoli = WattxHzxrad/moli]$ are compared with *Plank-Einstain* equation $E^{P1} = \Delta\delta x\omega xhxN_A[Jx10^{-6}xrad/moli]$. Continues transformation from torus to rectangle (f), and from rectangle to torus (f^1), is a homotopic process, able to used polyhedron number in rad or radieni (π). The wave character of NMR data shown interesting relationship between angles on 3-Sphere units approach. Bond distances $l_{CnCn+1}[A^0]$ of five membered ring iminocyclitols 1, 2 are calculated from dihedral angles θ_{HnHn+1}[deg]. Methods for calculation of the vicinal coupling constant $^3J_{HH}$ [Hz] with 3-Sphere – Polar equation – Conic section - Lie algebra - Hopf fibration, are disclosed from the mathematic point of view and in *far field* from physics electromagnetic radiation point of view.

Keywords: Graph Flux Intensity, Electromagnetic Wave, Vicinal Coupling Constant $^3J_{HH}$ [Hz], 3-Sphere, Hopf Fibration, Conic Section, Rectangle, Carnot's Theorem, Homotopic

1. Introduction

The wave character of NMR data enables calculation of the physical properties of iminocyclitols using varies transformation. Since the mathematics and physics rules are found on the whole nature world, *i.e.* the surface of polyhedron are governed by the Fibonacci number [1], and as well known the iminocyclitols are inscribed on polyhedron geometries. The dodecahedron dual icosahedron polyhedral are surface structural motif of five and six membered ring carbasugar, usefully geometries for calculation of the tetrahedral angles. [1] 3-Sphere theory enable calculation of the dihedral – vicinal angles [2] and tetrahedral – internal [1, 3-5] angles from chemical shift, a way to translate the wave character of NMR data in physical and at list in stereochemical information. Only from vicinal coupling constants can be calculated dihedral angles. [6, 7] From carbon and/or proton chemical shift the higher dimension characteristic for *cis/trans* stereochemistry can be solved with manifold equations [2, 8-10], trigonometric [2, 11-13] and algebraic approach [2], for calculation of three characteristic angles tetrahedral – dihedral – vicinal.

3-Sphere, also namely glome, analogue of a sphere is a higher-dimension space, embedded in 4-dimensional Euclidean space as the set of points equidistant from a fixed central point. Since the boundary of a ball in three dimensions is a 2-sphere in two-dimensional surface, the boundary of a ball in four dimensions is a three-dimensional manifold, as demonstrated in 2003 by Grigori Perelman, with Poincaré conjecture. Spherical 3-manifold is fundamental group, a binary icosahedral group of order 120. The space R^4 is preferably considered a space with 2 complex dimensions (C^2) or quaternions (H). The unit circle is characteristics for polar coordinates, in case of 3-sphere the 4-dimensional space in polar coordinates involved quaternion multiplication. Georges Lemaitre elliptic space is at base of 3-sphere theory. [14]

Hypersphere coordinates:

$X_0 = r\cos\psi$

$X_1 = r\sin\psi\cos\theta$

$X_2 = r\sin\psi\sin\theta\cos\varphi$

$X_3 = r\sin\psi\sin\theta\sin\varphi$

In two-complex dimensions $(z_1, z_2) \in C^2$:

$z_1 = e^{i\xi}_1\sin\eta$

$z_2 = e^{i\xi2}\sin\eta$

Expressed in R^4 as Hopf bundle $S^1 \rightarrow S^3 \rightarrow S^2$:

$X_0 = \cos\xi_1\sin\eta$

$X_1 = \sin\xi_1\sin\eta$

$X_2 = \cos\xi_2\cos\eta$

$X_3 = \sin\xi_2\cos\eta$

The stereochemistry of dihedral angles calculated from NMR data fit well on 3-Sphere theories with hypersphere coordinates [11, 12] or Hopf bundle [2]. Conformational analysis on five [15] and six [16] membered ring, Altona map [17] *versus* VISION Molecular model, was performed with 3-Sphere torsional angles [16].

From physics electromagnetic radiation point of view in *far field* result concentric circles [14], from mathematics 3-sphere theories [2], three concentric cons are easy to translate from higher dimension space in 2D, respectively in two sets angles, set A – dihedral angles θ_{HnHn+1} [deg], set B – vicinal angles ϕ [deg], angle result from vicinal coupling constant $^3J_{HnHn+1}$ [Hz].

2. Dihedral Angles Calculation with Graph Flux Intensity and Electromagnetic Wave

2.1. Graph Flux Intensity and Electromagnetic Wave

The magnetic field in gauss (eq. 1) and graph-flux intensity (eq. 2 - 4) gives almost equal characteristics angles as demonstrated with golden ratio eq. 5. [8, 18] The magnetic field is equal with the electric field if factor of correction is applied; B ~ E (eq. 7), with the angle obtain from one of them under the 3-sphere unit rule [2] can be calculated the dihedral angle θ_{HnHn+1} [deg] in close relationships with vicinal constant couplings $^3J_{HH}$ [Hz] from the differences between two atoms of carbon chemical shift $\Delta\delta_{CnCn+1}$. Six possible torsional

angles with *cis*- and *trans*-stereochemistry are represented on three concentric cones are translate from 3D to 2D introducing six sets angles (units U and S, both on unit C result from sin function or unit T result from tan function), or seven sets angles, ensuring right stereochemistry. [7, 18]

Magnetic field [2, 8]: $B = \nu x 4\pi x 10^{-3}/\gamma$ [gaussx10]

$$= \delta x 7.0028 x 4\pi x 10^{-3} [Tx10^{-3}] \quad (1)$$

where: ν – frequency [Hz], $\nu = \delta x \omega_L$: ω_L– Larmor frequency [^{13}C: 75MHz], δ_{Cn} – chemical shifts [ppm], γ – gyromagnetic ratio: ^{13}C: $\gamma = 10.71$ [MHzxT^{-1}] $= 6.7$ [10^7xradxT^{-1}xs^{-1}].

Intensity of magnetic field: $B_o = 2\pi x \omega_L/\gamma$ [MHzxT^{-1}] $= 2\pi x 75/10.71 = 7.0028$ [T], 1 [T] $= 10^4$ [gauss] $= 10^3$ [A/m]; $B = \mu H$ [oersted]; where H - field intensity, B – magnetic field [gauss], 1 [oersted] $= 10^3/4\pi$ [A/m], μ – magnetic permeability.

Graph-flux intensity [18, 8]: $E^G = E^n/1.54$ [graf/A^0] (2)

where n = GI, GII

Graph energy: $E^{GI} = \nu/628$ (3)

Pentagon golden ratio: $E^{GII} = \nu/682.787444$ (4)

Golden ratio [18]: $\{[1 + (5)^{1/2}]/n\}^{n+m} = Ox(1.6180)^{n+m}$ (5)

Pentagon: n = 5, m = 10:

$$\{[1 + (5)^{1/2}]/n\}^{15} = 1/682.787444 \quad (6)$$

$$E^{GI} \sim 4xE^{P1}/10^{-6} \quad (7)$$

$$f^G = 682.7874443/628 = 1.087241153 \quad (8)$$

The absorption of radio wave in the presence of magnetic field gives information about the electronic structure of molecule, the resonance frequency on Plank equation E = vxh [J] (eq. 9) transformed in E = $\Delta\delta x \omega x h x N_A$ [J/molix10^{-6}] (eq. 11) enable calculation of the dihedral angles also under 3-sphere approach. The cube of frequency ν [Hz] (eq. 13) enable calculation of the energy in WattxHz. Spectral flux [W/Hz], the radiant flux per unit (1erg = 10^{-7} [Wxs]), in this case become W/s.

The energy of radio frequency (rf) radiation [8]:

$$\text{Plank: } E = \nu x h \text{ [J]} \quad (9)$$

Plank-Einstain: E = mxc^2 = hxc/λ, λ = c/ν, E = $\nu x h$ (10)

where: ν – frequency of radio waves lies between 10^7 and 10^8 [cps], [1cps = 1Hz = cycles/sec]

h - Plank's constant;

$$E^{P1} = \Delta\delta x \omega x h x N_A/n \text{ [Jx10}^{-6}\text{xrad/molixn]} \quad (11)$$

with Plank constant h = 6.626070080x10^{-34} [Jxsxrad],

Avogadro $N_A = 6.023x10^{23}$ [moli^{-1}], n = 1 or n =1.54[A^0].

Electric energy:

Power – torque-scalar product – angular velocity [14]:

$$P = \tau.2\pi.\nu \quad (12)$$

where: [N.m] - cross product of force and distance or [J/radian] - energy per angle;

[J/rad]x [rad/rev]x [rev/sec] = [J/s] = [W]

[J/s] = [W], the unit of radiant power: [W/A^0]

Angular momentum [14]$:$ $\tau = rF\sin\theta$ (13)

τ – torque: has dimension force times distance [L^{2}MT^{-2}]

$$E^{P2} = (\Delta\delta x\omega)^2 xhxN_A/n = (\nu)^2 xhxN_A/n \quad (14)$$

where: $[1/s]^2 x[Jxsxrad]x[moli^{-1}]/n = [Jx10^{-3}xrad/sxmolixn] = [Wx10^{-3}rad/ molixn]$, n = 1 or n = 1.54[A^0].

$$E^{P3} = (\Delta\delta x\omega)^3 xhxN_A/n = (\nu)^3 xhxN_A/n \quad (15)$$

where: $[1/s]^3 x[Jxsxrad]/[molixn = [Jxrad/s^2xmolixn] = [Wxrad/sxmolixn] = [WxHzxrad/molixn] = [JxHz^2xrad/molixn]$, n = 1 or n = 1.54[A^0].

Plank constant h-bar result from h divided with 6.2799 rad:

$$E\text{-bar} = \Delta\delta x\omega xh\text{-bar}xN_A/n \; [Jx10^{-6}x\pi/moli] \quad (16)$$

where: h-bar = 1.055106713x10^{-34} [Jxsxπ].

In table 1, dihedral angles θ_{HnHn+1} [deg] and its corresponding vicinal coupling constants $^3J_{HH}$ [Hz] of iminocyclitols 1, 2 [20] (Figure 1) are calculated from the differences between two atoms of carbon consecutives with eq.

3, 4, 11, 15 and then divided or multiplied with 3, 6 or 9, in function of the values of calculated energy and its invers function. The number 3, 6, 9 remembered by the Tesla's numbers. In case of fractional absorption, after beam passes through the first layer the initial energy E_0 is reduced to $E_0/3$, at second layer to $E_0/9$, at third layer to $E_0/27$ [21]. With all equation are obtained values of the vicinal coupling constant $^3J_{HH}^{calc}$ [Hz] almost equals with recorded $^3J_{HH}^{exp}$ [Hz], and determined the factor of correction between the unit of radiant power [W/A^0] and pentagon golden ratio energy E^{IIG} in comparation with the graph energy E^{IG}. The magic angle result from the differences between pentagon golden ratio and graph: 682.7874 – 628 = 54.78744 [deg], the correlation between the eq. 3 and eq. 11: $E^{GI} \sim 4xE^{P1}/10^{-6}$ (eq. 7).
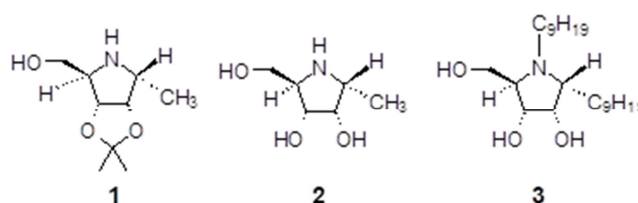

Figure 1. *Iminocyclitols with α-D ribitol (1, 2, 3) stereochemistry.*

Table 1. Dihedral angles θ_{HnHn+1} [deg] and vicinal coupling constant $^3J_{HnHn+1}$ [Hz] calculated with Graph-flux intensity (eq.2), graph energy (eq.3), pentagon golden ratio (eq.4), Plank eq. 11 - 15 (E = E^n/1.54, n = GI, GII, P1, P2, P3).

Entry	$^3J_{HH}^{exp}$ [Hz]	$\Delta\delta_{CnCn+1}^a$ [ppm] [Hz]	θ_{HH} [deg] $^3J_{HH}^{calc}$ [Hz] n	E^{GI}/1.54 [Graph/A^0]^f	E^{GII}/1.54 [Graph/A^0]^f	E^{P1}/1.54 [Jxrad/molixA^0]^f [4xE^{GI}/A^0]	E^{P2}/1.54 [Wxrad/molixA^0]^f	E^{P3}/1.54 [Wxrad/sxmolixA^0]^f
	1.							
			E	2.14813	1.97576	2.15355		2.32369
			Ex3	6.44439	5.92728	6.46066	1.1185014	6.97107
1.			1/Ex3	0.15517	0.16871	0.15478	E/6 0.149009	0.14344
	4.1	27.7	θ_{HH}	21.07	20.28	21.09	21.43	21.75
		2077.5	$^3J_{HH}$	4.15	4.17	4.15	4.14	4.13
			E/3				0.8940533	
			E/6	0.358021	0.32929	0.358925	-	0.387281
2.			θ_{HH}	20.9787	19.2259	21.0342	21.89	22.7854
			$^3J_{HH}$	4.15	4.20	4.15	4.12	4.09
			E	0.062039	0.05706	0.062196	0.932948	0.5597(10^{-4})
3.			Ex9	0.558358	0.513555	0.559768		
		0.8	θ_{HH}	-26.057	-29.09	-25.960	-26.697UtoS	-25.960
	5.4	60	$^3J_{HH}$	5.38	5.45	5.38	5.40	5.38
			E/3	0.020679	0.01902	0.02073	-	-
4.			θ_{HH}	-28.815	-28.9101	-28.8120		
			$^3J_{HH}$	5.45	5.45	5.45		
			E	0.09693	0.08915	0.09718	0.02277(10^{-6})	0.02135(10^{-2})
5.			E/3	0.03231	0.02971	0.03239		
			θ_{HH}	-28.148	-28.29	-28.14	-28.694	-28.77
			$^3J_{HH}$	5.43	5.43	5.43	5.44	5.44
			Ex3	0.290811	0.267476	0.291546	-	-
6.	5.4	1.25	θ_{HH}	-27.841	-26.914	-26.0988		
		93.75	$^3J_{HH}$	5.42	5.406	5.387		
			Ex6	0.58162	0.53495	0.58309	-	-
7.			θ_{HH}	-24.435	-27.659	-24.331		
			$^3J_{HH}$	5.35	5.42	5.34		
			E^{2}x6	0.05638	0.04769	0.05666	-	-
8.			θ_{HH}	-26.767	-27.266	-26.75		
			$^3J_{HH}$	5.40	5.41	5.40		
9.	0	18.4	E	1.42691	1.31241	1.43052	0.4935296	0.681070

Entry	$^3J_{HH}^{exp}$ [Hz]	$\Delta\delta_{CnCn+1}^{a}$ [ppm]	θ_{HH} [deg] $^3J_{HH}^{calc}$ [Hz] n	$E^{GI}/1.54$ [Graph/A⁰]^f	$E^{GII}/1.54$ [Graph/A⁰]^f	$E^{P1}/1.54$ [Jxrad/molixA⁰]^f [4xE^GI/A⁰]	$E^{P2}/1.54$ [Wxrad/molixA⁰]^f	$E^{P3}/1.54$ [Wxrad/sxmolixA⁰]^f
		1380	1/Ex9	0.07786	0.08466	0.07767	-	E/9: 0.075674
			θ_{HH}	85.533	85.143	85.143	89.572	85.660
			$^3J_{HH}$	1.056	1.101	1.101	0.326	1.041
			1/E	0.70081	0.76195	0.69904		E: 0.68107
10.			θ_{HH}	88.989	80.726	88.701		85.854
			$^3J_{HH}$	0.503	1.522	0.569		1.018
	2.		E	1.09345	1.00571	1.09621	0.2898116	0.306475
			1/E	0.91453	0.99451	0.91223	0.8694349^d	0.919427^d
11.	3.1	14.1 1057.5	1/Ex6	0.15242	0.16571	0.152038	0.1449058	0.153237
			θ_{HH}	51.232	50.460	51.254	51.668	51.185
			$^3J_{HH}$	3.11	3.14	3.11	3.09	3.11
		0.2	E	0.01550	0.01426	0.01554	0.0583092	$0.87463(10^{-6})$
12.	3.9	15	θ_{HH}	29.11	29.182	29.109	29.216	28.997
			$^3J_{HH}$	3.9	3.89	3.9	3.89	3.90
			E	0.38774	0.3566	0.38872	$0.364432(10^{-4})$	0.01366
13.	3.9	5 375	E/9	0.04308	0.039626	0.04319	0.040492	
			θ_{HH}	27.530	27.728	27.524	27.67931	29.2169
			$^3J_{HH}$	3.95	3.94	3.95	3.947	3.89
			E Ex27	0.38076	0.35021	0.38173	$0.351431(10^{-4})$	0.012941^e 0.349419
14.	8.8	4.91 368.25	θ_{HH}	168.809^D	169.74^D	168.77^D	169.712^D	169.774^D
			$^3J_{HH}$	8.87	8.93	8.87	8.92	8.93

[a] 1. δ CDCl₃, ppm; 2. δ D₂0, ppm: ^{13}C 75 [MHz], γ 10.71 [MHzxT⁻¹], ^1H 400 [MHz], γ 42.58 [MHzxT⁻¹], [b] E^{P1} = [Jxrad/molix10⁶], [c] E^{P3} = [JxHz²rad/moli], [d] Ex3, Ex3/6; [e] E = 0.012941, sinE = 0.7415, S to U 169.75 [deg], 8.93 [Hz]; [f] 1.54[A⁰] *versus* 1.57[rad]: in first case golden ratio of pentagon (eq. 4) is divided with theoretic values of l_{CnCn+1}[A⁰] and compared with eq. 3, 11, 14, 15. In second case, 1.57[rad] can be considered the best transformation relative to eq. 3, 11, 14, 15.

The values of the dihedral angle were obtained directly from $E^{GI}/6$, relative to $1/E^{GI}x3$, but in both cases results almost equals (Table 1, entry 1, 2). The calculated vicinal coupling constants of *trans-ee* H_3H_4 around 1.1 [Hz] directly from 1/Ex9 is preferably to be replaced with 1/E, since the proton chemical shift of H_3 is doublet at 4.38 [ppm], as well the vicinal coupling constant is almost equal with 0 [Hz] (Table 1, entry 9). From 1/E result vicinal coupling constants around 0.5 [Hz] from set C of unit U1 or set B of unit U2 (Table 1, entry 10).

$$r = 1.57\cos^{1/2}(\theta/m)[rad] \quad (17)$$

$$l_{CnCn+1} = (l^0 xr)^{1/2}[A^0] \quad (18)$$

cis, trans^{6,1}- θ_{HnHm}: m = 1, *cis, trans*^{5,2}- θ_{HnHm}: m = 2

$\theta_{H3H4}^{trans-ee3,2}$: r = 1.57\cos^{1/2}(\phi)$ or m = 4

where: r - bond distance in rad, l_{CnCn+1} − bond distance in angstroms A⁰, l^0 – theoretic bond distance of C_nC_{n+1}, 1.54[A⁰], θ_{HnHn+1} − dihedral angle [deg]

Table 2. *Bond distances* $l_{CnCn+1}[A^0]$ *of five membered ring iminocyclitols 1, 2.*

Entry	δ_{Cn} [ppm]	$^3J_{HnHn+1}^{exp}$ [Hz]	nxR_{mC} [gaussx10]	θ_{HnHm} [deg]	$^3J_{HnHn+1}^{calc}$ [Hz]	r [rad]	l_{CnCn+1} [A⁰]
1.	1-C₁: 55.8		n 1/2: 0.38795	$\theta_{H1H2}^{cis-6,1}$: 22.827	4.09	1.50726	1.52354
2.	1-C₂: 83.5	H₁H₂: 4.1	n 2: 0.044817	$\theta_{H1H2}^{cis-6,1}$: -27.431	5.41	1.479108	1.50924
		H₂H₃: 5.4	n 1: 0.224089^a	$\theta_{H1H2}^{cis-6,1}$: -25.888	5.38	1.489141	1.51435
3.	1-C₃: 84.3	H₃H₄: 0		$\theta_{H3H4}^{trans-ee3,2}$:		1.569981^c	1.55491
			n 2: 0.257703		0.315		
4.	1-C₄: 65.9			θ^U 14.9338, θ^S -89.6028^b		1.509603	1.524725
5.	2-C₁: 57.4		n 2: 0.789915	$\theta_{H1H2}^{cis-5,2}$: 52.1776	3.07	1.48787	1.51371
6.	2-C₂: 71.5	H₁H₂: 3.1	n 1: 0.0056	$\theta_{H2H3}^{cis-6,1}$: 29.6790	3.88	1.46339	1.50120
			n 1/2: 0.028^a	$\theta_{H2H3}^{cis-6,1}$: 28.3948	3.92	1.472532	1.50588
7.	2-C₃: 71.7	H₂H₃: 3.9	n 1: 0.13725	$\theta_{H3H4}^{trans-6,1}$: -168.57^e	8.86	1.55435	1.54716
		H₃H₄: 8.8		$\theta_{H3H4}^{trans-6,1}$: -168.94^{setF}	8.88	1.55536	1.54766
8.	2-C₄: 66.8		n 1/2:	$\theta_{H3H4}^{trans-6,1}$: -165.932	8.71	1.546279	1.54313

[a] Rmc [gauss]; [b] θ^U 14.9338[deg], $\theta^S = 2x(3x\theta^U)$[deg]; [c] r = 1.57\cos^{1/2}(\phi); [d] m = 4; [e] conic section cap. 3.2.

In table 2 are calculated bond distances $l_{CnCn+1}[A^0]$ of five membered ring iminocyclitols 1, 2 from dihedral angles θ_{HnHn+1}[deg] with eq. 17 and 18 for *cis, trans*[6,1] and *cis, trans*[5,2] stereochemistry. In case of *trans-ee* stereochemistry must be used the vicinal angle φ[deg], angle result from vicinal coupling constant $^3J_{HH}$[Hz], [7, 16] alternatively m = 2 in eq. 16. Dihedral angles θ_{HnHn+1}[deg] are calculated from the differences between two atoms of carbon consecutives $\Delta\delta_{CnCn+1}$[ppm] with eq. 1. The transformation from unit U to unit S: $\theta^S = 2 \times (3 \times \theta^U)$[deg] giving the dihedral angle $\theta_{H3H4}^{trans-ee3,2}$ -89.6028[deg], with its corresponding vicinal angle φ 0.3971[deg]. Dihedral angles θ_{H3H4}[deg] with *trans-aa*[6,1] stereochemistry are calculated using conic section approach presented in cap.3.2 (-168.57[deg]) and units with seven sets angles (-168.94[deg], -165.932[deg]).

2.2. Homotopic Approach

Continues transformation from torus to rectangle (f), and from rectangle to torus (f^{-1}), is a homotopic process [12]. For example, the transformation from 57.3248/360 = 0.15915 [rad/s] in 6.283182 [s/rad]. The transformation from ppm in gauss, the calculation of the intensity of magnetic field don't used rad (eq. 1), the preferred value of the Plank constant is h and no h-bar, continuum transformation in f and f^{-1} probably solve the differences.

Between h and h-bar in case of calculation of the tetrahedral angles as presented in table 2 all the values remain in dodecahedron – icosahedron – golden ration range, with one observation with h dodecahedron value will be calculated at C_1 and with h-bar at C_4 (1-E_{C1}: 0.2659528 – $3.760064^{1/2}$ – 1.939088).

$$\sin^{-1}1/E^n = \varphi, \; n = ½, 1, 2 \tag{19}$$

Vicinal angle φ and vicinal coupling constant $^3J_{HnHn+1}$ [Hz] can be calculated from tan function with eq. 20, or *vice versa* with eq. 18.

$$\tan^{-1}1/E_n = \theta \rightarrow \varphi \rightarrow {}^3J_{HH} \text{ [Hz]} \tag{20}$$

Polyhedron eq. 21 with P in π, rad even deg under wave character of NMR data, and 3-Sphere theories with its unit's system of distribution of the dihedral – vicinal -tetrahedral -internal angles.

$$\tan A/2 = P = 2\sin B/2 \tag{21}$$

where A, B – angles in [deg]

In table 3 are calculated tetrahedral angles with eq. 11 (n = 1) for iminocyclitols 1-3 (Figure 2) in comparison with eq. 16, Plank constant h *versus* h-bar, in fact a borderline approach between Fibonacci and Plank constant, between mathematics and physics. For example, for 1-C_1 in first case the polyhedron number is 1.6702 (close to dodecahedron)[1] relative to 3.76006 ($E^{1/2}$ 1.93908), tetrahedral angles resulting from 1/E and $1/E^{1/2}$ (entry 1)..

Table 3. *Tetrahedral and dihedral angles of five membered ring iminocyclitols 1-3 calculated with eq. 11 and 16, Fibonacci versus Plank constants.*

Entry	δ_{Cn} [ppm]	$^3J_{HH}$ [Hz]	$E^{P1} = (\Delta\delta x\omega)xhxN_A$[b] $[Jx10^{-6}xrad/moli]$, φ_{Cn}[c][deg]	$E^{P1} = (\Delta\delta x\omega)xh\text{-}barxN_A$ $[Jx10^{-6}x\pi/moli]$, φ_{Cn}[c][deg]
1.	1-C_1: 55.8		$1.670210(x10^{-6})$, 1/E: 106.442^S	3.760064 1.93908, $1/E^{1/2}$: 106.202^S
2.	1-C_2: 83.5		$2.49932(x10^{-6})$, $1/E^{1/2}$: 101.524^S	2.512713, $1/E^{1/2}$: 101.773^S
3.	1-C_3: 84.3	H_1H_2: 4.1	$2.53360(x10^{-6})$, $1/E^{1/2}$: 102.158^S	2.488603, $1/E^{1/2}$: 101.327^S
4.	1-C_4: 65.9	H_2H_3: 5.2 H_3H_4: 0	$1.972524(x10^{-6})$, 1/E: 107.64^{S,P} 108.99^T	3.1837875, 1.7843171, $E^{1/2}$: 106.847^{S,P} 1.490139^d, 1/E: 106.62^S
5.	1-NH: 2.64		0.4214371, 1/E: 112.852^T 2.3728331, $1/E^{1/2}$: 110.052	1/E: 112.27^T 0.0671078, 1/E: 107.584^S
6.	2-C_1: 57.4		1.7180747, 1/E: 108.817^S	3.655254, 1.911871, $1/E^{1/2}$: 108.19^S
7.	2-C_2: 71.5		2.14011047, $1/E^2$: 102.611^S	2.934427, $1/E^{1/4}$: 104.44^{Se} 101.55
8.	2-C_3: 71.7	H_1H_2: 3.1 H_2H_3: 3.9	2.1460968, $1/E^2$: 102.539^S	2.9262424, $1/E^{1/4}$: 104.39^S 101.58
9.	2-C_4: 66.8	H_3H_4: 8.8	1.9994318, $1/E^2$: 107.598^{S,P} 1/E: 105.531^S	3.1408921, $1/E^{1/4}$: 105.71^S 100.74
10.	2-NH: 3.33		0.5315854, $1/E^2$: 106.414^S 1.8811649, $1/E^{1/2}$: 107.69^S	0.084647, $1/E^{1/2}$: 114.71^S $1/E^{1/4}$: 107.24^S
11.	3-C_1: 63.7		1.90664388, 1/E: 108.52^S $1/E^2$: 105.96^S	3.2937447, 0.3036057, 1/E: 107.67^S
12.	3-C_2: 72.5	H_1H_2: 4.8	2.17004209, $1/E^2$: 102.26^S	2.8939530, 0.3455481, $1/E^{1/4}$: 100.11^S
13.	3-C_3: 74.0	H_2H_3: 5.2 H_3H_4: 0	2.21493951, $1/E^2$: 101.76^S	2.8352918, 0.3526973, $1/E^{1/4}$: 100.82^S
14.	3-C_4: 69.3		2.07426092, $1/E^2$: 107.62^S	3.0275843, 0.3302963, 1/E: 109.28

[a] δ_C[ppm], ^{13}C 75 [MHz], γ 10.71 [MHzxT^{-1}]: **1**-CDCl$_3$, **2**-D$_2$O, 3-CDCl$_3$, [b] P = Dodecahedron: 1.6180339887, Icosahedron: 2.618033985; [c] S – sin, T – tan, P – polyhedron eq. 21: $\tan A/2 = P = 2\sin C/2$; [d] 10^{-7}; [e] $2\tan^{-1}x2\sin(180 - 104.44)/2$ (eq. 26).

From the transformation point of view, h-bar must be used for calculation of the energy from carbon chemical shift, but values obtained from h gives a symmetry characteristic to polyhedron angles, certainly the wave character enable large number of inversions under polyhedron equation once an angle is transformed in its isomer, approach which is out of rule in case of transformation from rad in radieni (π). Data presented in table 4 are calculated with eq. 15 for iminocyclitol 1, the transformation from Hz in W/s (E^{P3} Wxrad/sxmolixn), having as advantage the missing value of 10^{-6}, under the Fibonacci approach resulting both angles, respectively the expected tetrahedral angle for C_n analyzed and its angle of the pseudorotation, result point out recently [1] using three characteristic equations for determination of the isomers of tetrahedral angles also under Fibonacci approach.

Relationships between angles of polyhedron and its pentagon unit (eq. 22 – 27):

$$2 \times \sin^{-1}(1.61803395/2) = 107.99 \ [deg] \qquad (22)$$

$$2 \times \tan^{-1}(1/1.61803395) = 116.56 \ [deg] \qquad (23)$$

$$2 \times \cos^{-1}(1/1.61803395) = 103.65 \ [deg] \qquad (24)$$

$$\tan^{-1}(1.61803395)^2 = 69.09 \ [deg], \ 110.905 \ [deg] \qquad (25)$$

$$2 \times \tan^{-1}\{2 \times \sin \ [(180 - \theta)/2]\} = \sim 100 \ [deg] \qquad (26)$$

$$2 \times \sin^{-1}\{ \ [1/(\sin \ [(180 - \theta)/2])]/2\} = \sim 106 \ [deg] \qquad (27)$$

with $\theta \sim 103$ -105 [deg]

Table 4. Tetrahedral φ_{Cn} [deg], dihedral angles θ_{HnHn+1} [deg] and vicinal coupling constant $^3J_{HH}$ [Hz] of five membered ring iminocyclitols 1, 2 calculated with eq. 15.

Entry	δ_{Cn} [ppm]	$^3J_{HnHn+1}$ [Hz]	E [W/sxmolixπ]	Φ [deg]	$\varphi_{Cn}, \varphi_{Cn+1}$ [deg] θ_{HnHn+1} [deg], $^3J_{HnHn+1}$ [Hz]	φ^b [deg]
1.	1-C_1: 55.8		4.6579586	E: 102.397 $E^{1/4}$: 107.402	107.402, 102.598 21.299, 4.12	107.121
2.	1-C_2: 83.5	H_1H_2: 4.1	1.5608187 (x10)	E: 100.313 $E^{1/2}$: 106.342	100.313, 109.687 -29.06. 5.45	101.158
3.	1-C_3: 84.3	H_2H_3: 5.4 H_3H_4: 0	1.60611171 (x10)	E: 102.984 106.845^c $E^{1/2}$: 104.196	102.984, 107.016 -25.987, 5.58	100.594
4.	1-C_4: 65.9		7.6727185	$E^{1/4}$: 106.139 $E^{1/8}$: 101.635	106.139, 103.861 82.722, 0754	108.465
5.	2-C_1: 57.4		5.0702422	E: 101.374 $E^{1/2}$: 107.391 $E^{1/4}$: 106.239	107.391, 102.609 51.30, 3.11 106.329, 103.67 51.83, 3.088	106.839
6.	2-C_2: 71.5	H_1H_2: 3.1	9.7996634	E: 106.5391 102.629$^{eq.25a}$	102.62, 107.37 25.25, 4.023	$E^{1/4}$: 104.711^b 101.388
7.	2-C_3: 71.7	H_2H_3: 3.9 H_3H_4: 8.8	9.8821287	E: 106.56513 102.817$^{eq.25}$	102.817, 107.183 25.633, 4.011	$E^{1/4}$: 104.711^b 101.388
8.	2-C_4: 66.8		7.9913917	E: 105.822 102.370$^{eq.25}$ $E^{1/4}$: 107.008 $E^{1/8}$: 100.925	105.82, 104.178 165.82, 8.7 107.008, 102.99 167.007, 8.77	108.247

[a] $E_c = (\Delta\delta \times \omega)^3 \times$h-barx$N_A = [v]^3 \times$h-barx$N_A$ [Jxπ/s^{2}xmoli] or [Wxπ/sxmoli], [b] Eq., *Rev. Roum. Chim.,* 2023, 68(3-4), 187; DOI: 10.33224/rrch.2023.68.3-4.08.

Table 5. Dihedral angles θ_{HnHn+1} [deg] and vicinal constant couplings $^3J_{HH}$ [Hz] calculates from f and f^1 for iminocyclitols 1, 2.

Entry	$^3J_{HH}$ [Hz]	$\Delta\delta_{CnCn+1}$ ^{a} [ppm] [Hz]	B f [deg]^b	Φ [deg]	θ_{HnHn+1} [deg] $^3J_{HH}$^{calc} [Hz]	f^1 [deg]^c	Φ [deg]	θ_{HnHn+1} [deg] $^3J_{HH}$^{calc} [Hz]
	1.							
1.	4.1	27.7 2077.5	0.775910 69.831	69.831	ea^{1,6}: 20.168 4.17	115.992	68.014	ea^{1,6}: 21.98' 4.12^d
2.	5.4	0.8 60	0.022408 2.0168	117.983	ae^{1,6}: -27.98 5.43	44.6269	119.251	ae^{1,6}: -29.25 5.46
3.	5.4	1.25 93.75	0.035014 3.1512	116.848	ae^{1,6}: -26.84 5.404	28.5600	119.28	ae^{1,6}: -29.28 5.46
4.	0	18.4 1380	0.515406 46.3865^b	2.7731	ee^{1,4}: 92.22 0.83	174.619	5.3804 $_1^{A}$/2 2.2825	ee^{1,4}: 84.61 1.159 ee^{2,3}: 87.681 0.761
	2.							
5.	3.1	14.1 1057.5	0.394957 35.5462	35.54	ae^{2,5}: 54.45 2.98	132.127	35.744	ae^{2,5}: 54.25 2.98
6.	3.9	0.2	0.056022	65.042	ea^{1,6}: 24.95	17.8501	63.001	ea^{1,6}: 24.29

Entry	$^3J_{HH}$ [Hz]	$\Delta\delta_{CnCn+1}$[a] [ppm] [Hz]	B f [deg][b]	Φ [deg]	θ_{HnHn+1} [deg] $^3J_{HH}^{calc}$ [Hz]	f¹ [deg][c]	Φ [deg]	θ_{HnHn+1} [deg] $^3J_{HH}^{calc}$ [Hz]
7.	3.9	15 5 375	5.04201 0.140560 12.6504	64.699	4.03 ea[1,6]: 25.30 4.02	7.11439	63.557	4.05 ea[1,6]: 19.705 3.9
8.	8.8	4.91 368.25	0.137535 123.7815	77.621	aa[1,6]: 167.621 8.8	7.27087	78.557	aa[1,6]: 168.557 8.8

[a] 1. δ CDCl$_3$, ppm; 2. δ D$_2$0, ppm: ^{13}C 75 MHz, γ 10.71 [MHzxT^{-1}], [b] f = 2πv [Hz], [c] f¹ = 1/2πv [s], [d] θ$^{A'}$: φ$_1^C$/2.

Dihedral angles calculated with toric – rectangle approach, continuum transformation from torus to rectangle (f), and from rectangle to torus (f¹), having as intermediate a cylinder are presented in Table 5.

The invers of energy under 3-sphere approach: *i.e.* 1-$^3J_{H1H2}$ = 4.1 [Hz], $\Delta\delta_{C1C2}$ = 27.7 [ppm]: B = 0.7750 [gauss], 1/B = 1.2888 [1/gauss] resulting angles 69.831 [deg] and 115.994 [deg] with the corresponding dihedral angles 20.168 [deg] and 21.98 [deg], but not at list with φ$_{1/2}^B$ = φ$_2^{1/B}$.

An interesting example, the angles calculated from h with eq. 11 for n = 1 (E = vx39.9088200x(10^{-11})) and h-bar eq. 16 (E-bar = vx6.3516841(10^{-11})) can be found on two sets angles. For a differences in carbon chemical shift of 1-$\Delta\delta_{C1C2}$ 2077.5[Hz] are calculated angles 19.36^{A1} and 70.63^{B3}[deg] with eq. 28, 29 and angles 7.58^{A1}, 82.41^{B3}[deg] with eq. 30, 31. Building seven sets angles form angles calculated with h-bar, on sets F and G are found angles 18.79^{F1}, 71.20^{G3}[deg] approximately equals with angles calculated from h, and dihedral angle 22.41^{B1}[deg]. In first two sets angles calculated from h are found two angles 40.69^{A2} and 49.36^{B2}[deg] almost equals with angles 49.25^{A2} and 40.74^{B2}[deg] calculated from h-bar eq. 32, 33. Differences between the angles calculated with h and h-bar are ~ 0.1-0.57[deg]. Thus, angles calculated from h and h-bar are found on unit with seven sets angles along the dihedral angle. Alternatively, can be used eq. 34 and 35 with smaller differences, resulting in both cases angles approximately equals with eq. 28, 29. The Plank constant h-bar (eq. 16) is the most preferred for calculation dihedral angle θ$_{HnHn-1}$[deg], angle found in unit with seven sets angles, without transformation[2] from U to S and S to U(chapter 3.4).

$$\sin \theta^A = 1.5963xvx(10^{-9}) \quad (28)$$

$$\cos\theta^B = 1.5963xvx(10^{-9}) \quad (29)$$

$$\sin\theta^A = v/1.574x(10^{10}) \quad (30)$$

$$\cos\theta^B = v/1.574x(10^{10}) \quad (31)$$

$$\sin\theta^B = 1.574x(10^{-10})/v \quad (32)$$

$$\cos\theta^B = 1.574x(10^{-10})/v \quad (33)$$

$$P = vx[(1/hxN_A)/4] = vx6.26427x(10^8) \quad (34)$$

$$P\text{-bar} = vx[4x(1/h\text{-barx}N_A)] = vx6.29754x(10^{10}) \quad (35)$$

Another example useful for demonstrating the concept of homotopy, a rectangle with two sides equal with golden ratio (φ^G = 1.6180339884) and two sides equal with one, vertices of Platonic solids (Dodecahedron or Icosahedron), gives almost equals values of the pentagon internal angles from *cos* function of

φ^G and its invers 1/φ^G (2xcos^{-1}(φ^G/2) = 72.0000683 [deg]; 2xcos^{-1}(1/φ^G)/2 = 71.999999^{deg}, 2xcos^{-1}(1/φ^G) = 103.65 [deg]).

3. Methods for Calculation of the Vicinal Coupling Constant $^3J_{HH}$ [Hz] with 3-Sphere Manifold

3.1. 2D Rectangle Versus Polar Equation Approach for Calculation of the Vicinal Coupling Constant

As well as the symmetry of the geometric forms is found in the whole nature world, the chemistry is not out of the mathematic rule. The apple shape of the polar curve cardioid, a particular case of limaçons, was used also for the sign of chirality determination, the sign of chirality depending on the direction of the apple cut. [22] The direction of the DNA spiral used as an architectonic motif at the *"Curtea de Arges"* monastery. The pucker of the furanose ring in DNA was explained by Davis as a way to distinguished DNA in its two roles as a template for DNA in replication and for RNA in transcription. [23]

The polar coordinate system is similar to the rectangular coordinate system, with a series of circles extending out from the pole (or origin in a rectangular coordinate grid) and five different lines passing through the pole to represent the angles at which the exact values are known for the trigonometric function, system used for the construction of the Altona map. The circle, ellipse or sphere are known models used for the representation the deviation from the planarity in polar coordinates of the five and six membered ring.

In polar coordinate two classical curves explain well the generalized Karplus equation: 1. limaçons or cardioid, 2. rose or lemniscale. Three types of conics are known: the ellipse, parabola, hyperbola. The circle is a special case of ellipse, if the intersection of the cone and the plane is a closed curve occurs circle or ellipse. Invers of the conic: ellipse – limaçons with no loop, parabola – cardioids, hyperbola – limaçons with inner loop or Leniscate of Bernulli – if the inversion circles is centered at the center of the hyperbola, and Lookwood's equation. Transformation from ellipse to lemniscate of Bernulli, having as intermediate the Cassini oval, a special case of limaçons, point out the relationships between the polar equation, class of sinusoidal spiral. The cissoid ("ivy shaped") with two curves C$_1$ and C$_2$ and a point fixed O, can be: line, conchoid of Nicomedes, Conchoid of the Sluze, oblique cissoids, cissoids of Diocles, strophoid, circle, lemniscate. Conchoid of the Sluze: is the roulette of a parabola vertex. Cissoid of Diocles: is the cubic curve. [14]

3.1.1. 2D Rectangle

The vicinal coupling constant $^3J_{HH}$ [Hz] can be calculated from the differences between two atoms of carbon and two protons using 2D rectangle geometries (eq. 36) under homotopic approach, characteristic for wave field.

$$^3J_{HH} = [a + bxAx(a/b)]^{1/2} \qquad (36)$$

with A = cos, sin, cosec, tan, cotan; a = $\Delta\delta_{HnHn+1}$ or $1/\Delta\delta_{HnHn+1}$ [ppm], b = $\Delta\delta_{CnCn+1}$ or $1/\Delta\delta_{CnCn+1}$ [ppm].

Table 6. Dihedral angles of 2 calculated with Carnot's theorem (eq. 29).

Entry	H_nH_{n+1}	δ_{HH} [ppm]	$\Delta\delta_{HH}$ [ppm]	δ_{CC} [ppm]	$\Delta\delta_{CC}$ [ppm]	$^3J_{HH}^{exp}$ [Hz]	D d = θ or ϕ [deg]	$^3J_{HH}^{pred}$ [Hz]
1.	2-H_1H_2-*cis*	H-1 3.71 H-2 4.16	0.45	C-1 57.4 C-2 71.5	14.1	3.1	129.424 50.575	3.13
2.	2-H_2H_3-*cis*	H-2 4.16 H-3 4.26	0.1	C-1 71.5 C-2 71.7	0.22	3.9	0.6292 60.629 29.16	3.89
3.	2-H_3H_4-*trans*	H-3 4.26 H-4 3.58	0.68	C-1 71.71 C-2 66.8	4.91	8.8	17.332[a] -162.667 39.6073[a] -169.803	8.52 8.93

[a] $[17.332 \times 90]^{1/2} = 39.607$.

3.1.2. Carnot's Theorem [14]

This method is especially useful for triangles with abstract forms [14], triangles induced by Lie algebras, that otherwise have the same properties as usual triangles.

$$d = [R(R - 2r)]^{1/2} \qquad (37)$$

In table 6 dihedral angles are calculated with the Carnot's theorem (eq. 37) from differences in carbon $\Delta\delta_{CC}$ and proton $\Delta\delta_{HH}$ chemical shift (eq. 38). In case of iminocyclitol 2 dihedral angles and corresponding vicinal coupling constant $^3J_{HH}$ [Hz] result almost equals with the predicted angles only from the vicinal coupling constant. In line with polar equation, optimal results cannot be obtained with only one equation, the shape of one CC bond is different around the five membered ring.

$$\theta, \phi = [\Delta\delta_{CC}(\Delta\delta_{CC} - 2\Delta\delta_{HH}) \times 90]^{1/2} \qquad (38)$$

3.2. Conic Section Approach [18].

The vicinal coupling constant $^3J_{HH}$ [Hz] can be calculated from the differences in chemical shift between two atoms of carbon consecutives $\Delta\delta_{CnCn+1}$ [ppm] using *conic section* [18], where h – altitude of con and r – half of cone base diameter. Six dihedral angles with *cis*, *trans* stereochemistry on three concentric cons are easy translate on 2D.

$$r = \sin\phi = [(h^2 - 1)/h]^{1/2} \qquad (39)$$

$$\cos\theta = 1/h \qquad (40)$$

Characteristic for the 180-three concentric cones approach are ϕ_1 and ϕ_2 [deg], the first one ϕ_1 is the value between two *trans-ee* angles $\phi_1 = \theta^4 - \theta^3$ [deg], the second one $\phi_2 = 60 - 2\phi_1 = \theta^3 - \theta^2 = \theta^5 - \theta^4$ [deg], representing the value between the *trans-ee - cis* angles, or *trans-ee - trans-aa* angles (Figure 2).

From chemical shift $\Delta\delta_{CnCn+1}$ [ppm] transformed in gauss are calculated angles of set A and set B and build two sets angles (A and B), both having six angles with all *cis*, *trans* stereochemistry (Table 7). Then, from the first angle of set A or B will be calculated one angle of second sets A' or B'. In case of iminocyclitol 2 for a vicinal coupling constant of 8.8 [Hz] from set B with conic section eq. 42 was calculated the angle $\theta^{B'2}$ with a dihedral angle of *trans-aa* 168.56 [deg] and a vicinal coupling constant of 8.86 [Hz], relative to 9.0 and 8.24 [Hz] calculated for angles 172.09 and 157.90 [deg] with eq. 67 and 70 (chapter 3.4).

$$\cos\theta^{A(n-1)1} = h^{n-1} \qquad (41)$$

$$\theta^{An2} = [(1/h^{n-1})/2] \times 90 \qquad (42)$$

Generalized conic equations (eq. 41, 42) for calculation of the dihedral angle and the vicinal coupling constant from n sets angles.

The vicinal coupling constants are calculated with algebraic equations 43 - 49, equations demonstrated with root system Lie group in Euclidean space. The Weyl group of the A2 root system fitting well into the 60/120 rule of dihedral angles [18, 24, 16].

Table 7. Vicinal coupling constant 2-trans-aa $^3J_{H3H4}$ [Hz] calculated with conic section approach.

Set A	Set B	Set B'	$^3J_{HH}$ [Hz], θ_{HnHn+1} [deg]
cis θ^{A1}: 7.9052	*cis* θ^{B1}: 22.0947	*cis* $\theta^{B'1}$: 18.5667	
cis θ^{A2}: 52.0947	cis θ^{B2}: 37.9052	cis $\theta^{B'2}$: 48.5665	
trans-ee θ^{A3}: 67.9052	*trans-ee* θ^{B3}: 82.0947	*trans-ee* $\theta^{B'3}$: 71.4335	$^3J_{HH}^{exp}$ = 8.8 [Hz]
trans-ee θ^{A4}: 112.0947	*trans-ee* θ^{B4}: 97.9052	*trans-ee* $\theta^{B'4}$: 108.5665	θ_{HnHn+1} = 168.56 [deg]
trans-aa θ^{A5}: 127.9052	*trans-aa* θ^{B5}: 142.0947	*trans-aa* $\theta^{B'5}$: 131.4335	$^3J_{HH}^{calc}$ = 8.86 [Hz]
trans-aa θ^{A6}: 172.0947	*trans-aa* θ^{B6}: 157.9052	*trans-aa* $\theta^{B'6}$: 168.5665	
$R_m = (\Delta\delta_{CnCn+1} \times \omega \times 4\pi \times 10^{-3})/10.71 = 0.137535$ [gauss] for $\Delta\delta_{C3C4}$ = 4.91 [ppm], ω_C = 75 [MHz]			
Alternatively [18]: $R_m = (\Delta\delta_{CnCn+1} \times \omega \times 4\pi \times 10^{-3})/l^0$ [1/sxA^0], l^0 = 1.54 [A^0]			

Set A	Set B	Set B'	$^3J_{HH}$ [Hz], $\theta_{H_nH_{n+1}}$ [deg]
$R_m = \sin\theta^{An}$ $R_m = \cos\theta^{Bn}$ $n = 1 - 6$ $180 - \theta^{cis, trans} = \theta^{trans, cis}$ $\phi_{1A}/2 = 90 - \theta^{A3}$, $\phi_2 = \theta^{A3} - \theta^{A2}$, $\phi_{1B}/2 = 90 - \theta^{B3}$, $\phi_2 = \theta^{B3} - \theta^{B2}$	$\cos\theta^{A1} = h^1$ $\theta^{A'2} = [(1/h^1)/2]x90$ $\cos\theta^{B1} = h^1$ $\theta^{B'2} = [(1/h^1)/2]x90$	$\cos\theta^{A'1} = h^2$ $\theta^{A''2} = [(1/h^2)/2]x90$ $\cos\theta^{B'1} = h^2$ $\theta^{B''2} = [(1/h^2)/2]x90$	$\cos\theta^{A(n-1)1} = h^{n-1}$ $\theta^{An2} = [(1/h^{n-1})/2]x90$ $\cos\theta^{B(n-1)1} = h^{n-1}$ $\theta^{Bn2} = [(1/h^{n-1})/2]x90$

Algebraic equations 43 - 46 for positive dihedral angles with *cis*-, *trans*-stereochemistry:

cis/trans-aa^{6,1}:

$$^3J_{HH}{}^{aa6,1} = [(\phi_1 + \phi_2 + \phi_1/2)^n]/m = [(60 + \phi_1/2)^n]/m \quad (43)$$

cis/trans-aa^{5,2}:

$$^3J_{HH}{}^{aa5,2} = [(\phi_2 + \phi_1/2)^n]/m \quad (44)$$

cis/trans-ee^{3,2}:

$$^3J_{HH}{}^{ee3,2} = [(\phi_2{}^U - \phi_1{}^U/2)^n]/m = (\phi_1{}^S/2)^n/m \quad (45)$$

cis/trans-ee^{4,1}:

$$^3J_{HH}{}^{ee4,1} = (\phi_1{}^U/2)^n/m \quad (46)$$

Algebraic equations 38 - 40 for negative dihedral angles with *cis*-, *trans*-stereochemistry:

cis/trans-aa^{6,1}:

$$^3J_{HH}{}^{aa6,1} = [(120 - \phi_1/2)^n]/m \quad (47)$$

cis/trans-aa^{5,2}:

$$^3J_{HH}{}^{aa5,2} = [(120 + \phi_1/2)^n]/m \quad (48)$$

cis/trans-ee^{4,1}:

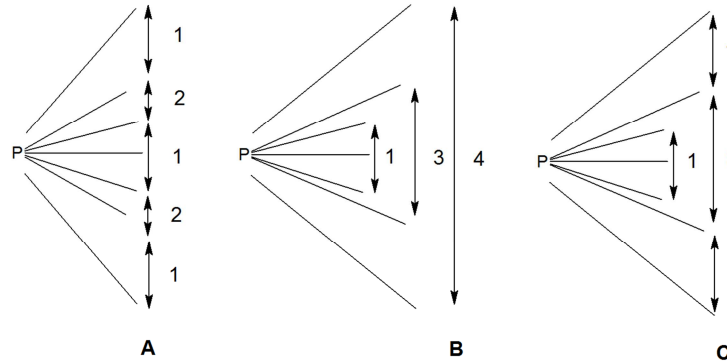$$^3J_{HH}{}^{ee4,1} = [(120 + \phi_2 + \phi_1/2)^n]/m \quad (49)$$

Figure 2. *Three 180-concentric cones diagrams for predicted cis (A) and trans-H_nH_m (B, C) dihedral angles (ϕ: 1, 2).*
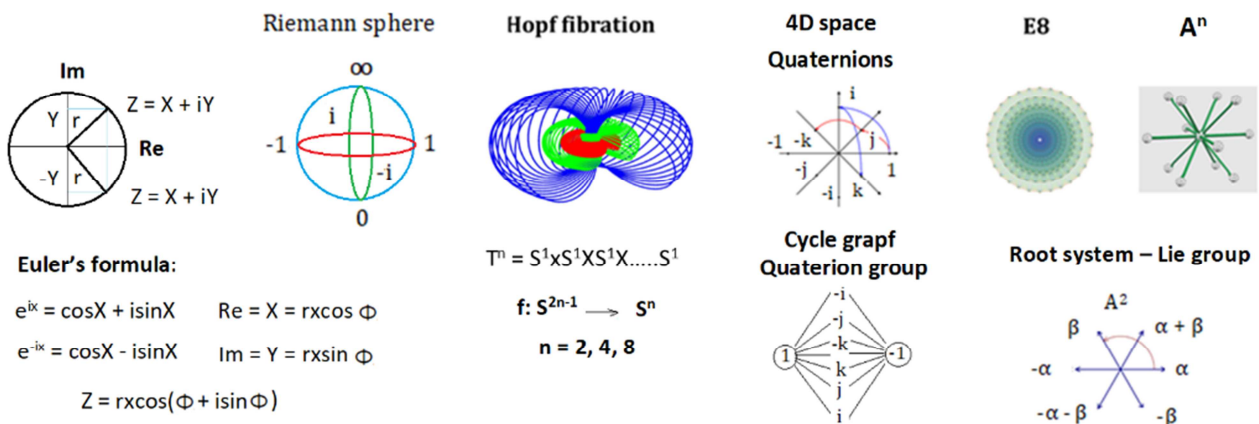

Figure 3. *Rienann sphere Quaternions-Hopf fibration and Root system-Lie group.*

3.3. Hückel – 3 Sphere Approach for Calculation of the Vicinal Coupling Constant [18]

Bloch sphere is a geometrical representation of the pure sate space of two-level quantum mechanical system (Qubit), mapped as Riemann sphere (eq. 50), in two-dimensional Hilbert space is the complex projective line CP1, 2-sphere unit known as Poincaré sphere. Mapped as 3-sphere unit, two-dimensional state space C^2 known as Hopf fibration.

$$I\psi> = \cos(\theta/2)I0> + e^{i\phi}\sin(\theta/2)I1> = \cos(\theta/2)I0> + (\cos\phi + i\sin\phi)\sin(\theta/2)I1> \quad (50)$$

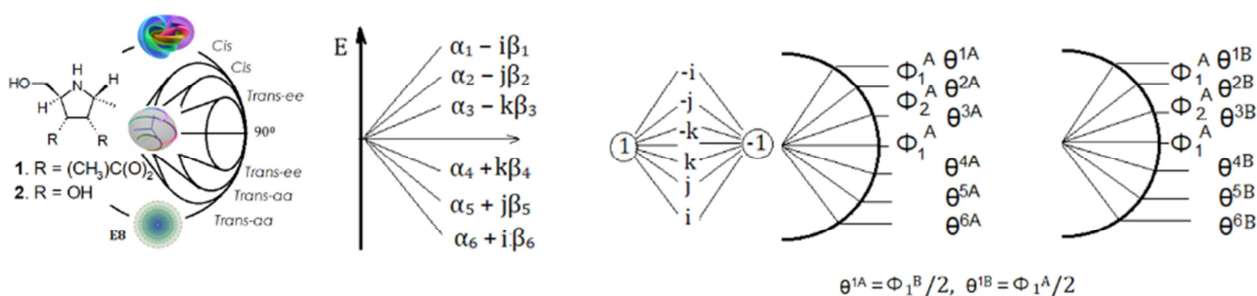with $0 <= \theta <= \pi$, $0 <= \phi < 2\pi$

Figure 4. Spherical representation in higher dimensional space with cyclic graph.

Hopf fibration required algebra of quaternions (Figure 3), solving the rotation of the 3-sphere in four dimensions space, with applications in electromagnetic wave. A torus can be mapped continuously to a finite plane, and a topological space that preserve homotopies give a fibration. The mapping f transform the torus into a plane, and the reverse map f^1 transform the plane into a torus. Hopf fibration having as key topologic structure a torus enables calculation of the vicinal angles in direct correlation with the vicinal constant couplings only from the differences between two atoms of carbon in two steps: 1. Set A is built from chemical shift δ [ppm] with one of manifold equation, 2. The vicinal constant coupling $^3J_{HH}$ [Hz] will be calculated using Hückel - Hopf fibration with eq. 51, 52 (Figure 4). The distribution of the m_x values between six possible torsional angles, from the stereochemistry point of view, gives information about the nature of the Hopf construction. The torsional angles are predicted in close relation with the vicinal constant coupling ($^3J_{HH}$), the best torsional angles having the values of predicted vicinal constant coupling closed to the recorded values.

The line bundles as topological structure underlying the electromagnetic field are known as "the magnetic monopole" (the Hopf fibration). The Hope fibration (η: $S^3 \rightarrow S^2$) describes 3-sphere (a hypersphere in four-dimensional space as a fibration $S^1 \rightarrow S^3 \rightarrow S^2$) in terms of circles ($S^1$ one-dimensional sphere) and on ordinary sphere (S^2 two dimensional sphere), in fact is a way to build three-sphere from a collection of circles drawn like points on a two-sphere. Each fiber is linked with each other fiber once. The collection of fibers over circles in S^2 is a torus ($S1 \times S1$). The Hopf construction produces the four Hopf fibrations: $S^0 \rightarrow S^1 \rightarrow S^1$ *real Hopf fibration,*

$S^1 \rightarrow S^3 \rightarrow S^2$ *complex Hopf fibration,* $S^3 \rightarrow S^7 \rightarrow S^4$ *quaterionic Hopf fibration (7-sphere over the 4-sphere with fiber the 3-sphere),* $S^7 \rightarrow S^{15} \rightarrow S^8$ *octonionic Hopf fibration (the 15-sphere over the 8-sphere with fiber the 7-sphere).* [14]

The vicinal constant couplings can be calculated from the differences between two angles from the same set $^3J_{HH} = f(\theta^{IA}, \theta^{IIB})$, with Hükel 1 (eq. 51) or Hükel 2 (eq. 52) [25, 26].

Hückel equation:

$$H1: E = \alpha + 2m_x x\beta \quad (51)$$

$$H2: E = \alpha + m_x x I 2\beta I \quad (52)$$

Where $m_x = \cos(2 x i x 180/n)$, $m_x = i, j, k$, $n = 0, -/+1/2, -/+2/2, -/+3/2, 1-7, 1-8, 1-4$.

The characteristic Hükel values m_x in Table 8 are calculated using spin quantum numbers, principal quantum numbers. Vicinal coupling constants are calculated in Table 9 for the differences between two atoms of carbon and two protons chemical shift with rectangle as manifold [9], two representative equations: skew circles and middle circles. This method was chosen because the dihedral angles or vicinal angles are in first set angles, relative to method for calculation of the dihedral angles only from the differences in carbon chemical shift, where the dihedral angle can be found on units. In first case the vicinal coupling constant was calculated from the differences between the angles having same stereochemistry as predicted dihedral angle, *i.e.* $^3J_{HnHn+1} = 3.1$ [Hz], $\Delta\theta = \theta^{B5} - \theta^{B2} = 82.080$ [deg], $^3J_{HnHn+1} = (82.080/1.2460)^{1/4} = 3.009$ [Hz].

Table 8. Values of m_x in radians.

Entry	J	n = 7 M1	J	n = 7 M2	J^c	n = 9 M3	J	n = 7 M4	n = 9 M5	n = 15 M6
1.	-1/2	1.80193	3	-1.80193	1	1.53208	2	-0.44504	0.34729	1.33826
2.	-2/2	1.24697	1	-0.44504	2	1.33826	3	-1.80193	-1	0.61803
3.	-3/2	0.44504	2	1.24697	3	-1	4	-1.80193	-1.8793	-0.20905
4.	0	1	7	1	4	-1.87938	1	1.24697	1.53208	1.82709
5.	3/2	0.44504	5	1.24697	5	-1.879389	1	1.24697	1.53208	1.82709
6.	2/2	1.24697	6	-0.44504	6	-1	4	1.80193	-1.8793	-0.20905
7.	1/2	1.80193	4	-1.80193	7	0.347296	3	1.537088	-1	0.61803
					8	1.537088	2	-0.44504	0.34729	1.33826

Table 9. *Dihedral θ_{HnHn+1} [deg] and vicinal coupling constant $^3J_{HnHn+1}$ [Hz] calculated with Hückel – 3 Sphere approach.*

Entry	$\Delta\delta_{HnHn+1}$ [ppm] $\Delta\delta_{CnCn+1}$ [ppm]	$^3J_{HnHn+1}^{exp}$ [Hz]	θ^{An} [deg] θ_{HnHn+1} [deg] ϕ [deg] $^3J_{HnHn+1}$ [Hz]	$\Delta\theta$ [deg] m_x $^3J_{HnHn+1}^{calc}$ [Hz] H1 (M1, 2) n 7	$\Delta\theta$ [deg] m_x $^3J_{HnHn+1}^{calc}$ [Hz] H1 (M3-6) n 7, 9, 15	$\Delta\theta$ [deg] m_x $^3J_{HnHn+1}^{calc}$ [Hz] H2 (M3-6) n 7, 9, 15
1.	1-H₁H₂: 1.41 1-C₁C₂: 27.7	4.1	83.84 23.84 66.16 4.06	297.290 0.44504 4.152	271.3352 0.61803 4.058 n 15	-
2.	1-H₂H₃: 0.11 1-C₂C₃: 0.8	5.4	11.14 -26.56 116.56 5.39	388.997 0.44504 4.441	828.1272 -0.209 5.364 n 15	-
3.	1-H₃H₄: 1.16 1-C₃C₄: 18.4	0.1 (d H₃)	58.88 -88.88 1.12 0.52	1.24005 1.80193 1.05526	-	1.2230 1.8270 0.743 n 15 1.18900 -1.87938 0.7383 n 9
4.	2-H₁H₂: 0.45 2-C₁C₂: 14.1	3.1	51.1761 38.823 3.1154	82.0801 1.24697 3.009	102.3523 -1 3.180 n 9 82.0808 1.24697 3.009 n 7	371.4310 -0.20905 3.104 n 15 294.712 0.3472 2.929 n 9
5.	2-H₂H₃: 0.1 2-C₂C₃: 0.2	3.9	1.89 28.10 61.9 3.93	261.110 0.44504 4.01	200.3058 0.61803 3.762 n 15	-
6.	2-H₃H₄: 0.68 2-C₃C₄: 4.8	8.8	12.24 -167.75 77.75 8.81	144.489 1.80193 8.95	76.8815 -1.87938 8.76 n 9 79.08203 1.82709 8.89 n 15	-

As observation, the vicinal coupling constant $^3J_{HnHn+1}$ [Hz] (eq. 53, 54) result from the set containing the vicinal angle ϕ [deg] or dihedral angle θ_{HnHn+1} [deg], in example presented result from the set containing vicinal angle. Octonionic Hopf fibration (n = 15) was calculated from angles of set containing the dihedral angle (Table 8, entry 4), quaterionic group Sp(2), Sp(1)cSO(8), the Spin(9)cSO(16) [27] for both Hükel 1 or Hükel 2 with n = 9, and also real Hopf fibration with n = 7.

Vicinal constant couplings:

$$\text{H1: } ^3J_{HH} = [\theta^{IA} - \theta^{IIA}]/m_x]^{1/n} \tag{53}$$

$$\text{H2: } ^3J_{HH} = \{[(\theta^{IA} - \theta^{IIA})/m_x]^{1/2}/2\}^{1/n} \tag{54}$$

n = 4 *cis*, n = 2 *trans*
I, II: 1, 6; 2, 5; 3, 4.

3.4. 3-Sphere Approach [2].

Poincare conjecture is a theory about 3-sphere, a hypersphere that bound the unit ball in four-dimensional space, were a point increase to circle and then is transforms to a torus. 4-Manifold was introduced by physicians' because in general relativity space - time is modeled as a pseudo-Riemannian 4-manifold.

Platonic solids or Catalan solids, with pentagon faces, are homeomorphic to the sphere. Poincaré dodecahedron space is binary icosahedral group of order 120. Topologically a ring torus is homeomorphic to the Cartesian product of two circles: $T^2 = S^1xS^1$, a compact 2-manifold of genus 1. Each distinct point of the two-sphere comes from a distinct circle of the three-sphere. Every point on the two-sphere produces a fiber that is a circle. Torus in 2D is a product of two circles – a modified version of the spherical coordinates system – having toroidal and poloidal coordinates, with cylindrical coordinates (and helices as geodesics), a limit case of the conic.

Six angles with *cis*, *trans* stereochemistry can be drawn on three concentric cons, in 2D one half circle with six angles having two characteristic angles ϕ_1 and ϕ_2 (Figure 5). From half ϕ_1^A result circle B, and from ϕ_2^A circle C. From first angles of sets A and B are builds other four sets angles resulting 7 sets units U or S. Six sets angles, three from U and three from S, ensuring relationship between dihedral and vicinal angles for all stereochemistry. Dihedral and vicinal angles can be found on two sets angles in close relationship with tetrahedral and internal angle, four sets angles which can

be found on seven sets angles on unit U or S or on six sets angles U and S. In unit S are found angles smaller as 5 [deg], as a general rule. Angle transformed from U to S with eq. 47

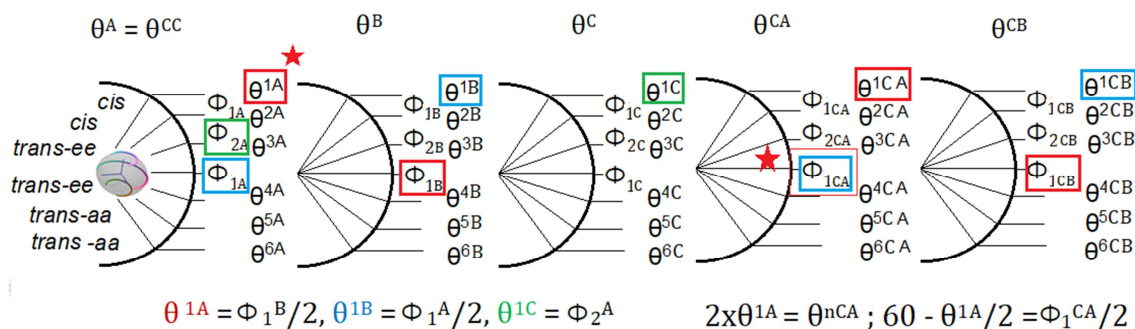are almost equals with angles calculated with tan trigonometric function.

Figure 5. *Three sets of possible torsional angles with cis- and trans-stereochemistry.*

Equations for transformation from S to U (eq. 55) and U to S (eq. 56):

$$S \text{ to } U: Z = [60 - (\theta^{S4} - 90)]/1.5 \qquad (55)$$

if $\theta^{S4} < 100$ result φ_1 or φ_4; $\theta^{S4} > 100$ result φ_2 or φ_3, where: φ_n – tetrahedral angles [deg], n =1-4, θ^{S4}- the fourth angle [deg] of sets A or B in unit S.

$$U \text{ to } S: Z = \phi_2^{U} - \phi_1^{U}/2 \qquad (56)$$

where: $\phi_1^{UA}/2 = \theta^{UB1}$ or $\phi_1^{UB}/2 = \theta^{UA1}$, $\phi_2^{UA} = \theta^{UC1}$ or $\phi_2^{UB} = \theta^{UC2}$, the algebraic angles [deg]: $\phi_2^{U} = \theta^{U3} - \theta^{U2}$, $\phi_1^{U}/2 = 90 - \theta^{U3}$, θ^{U3}, θ^{U2}- second and third angles [deg] of sets A or B in unit U.

Trans-ee[4,1]:

$$^3J_{HnHn+1} \sim \cos^{-1}[(\sin\phi)]^{1/2}/2 \qquad (57)$$

Where $\phi^{UA} = \phi_1^{UA}/2 = \theta^{UB1}$,
Trans-ee[3,2]:

$$^3J_{HnHn+1} \sim \tan^{-1}[(\sin\phi)]^{1/2}/2 \qquad (58)$$

Where $\phi^{UA} = \phi_2^{UA} - \phi_1^{UA}/2 = \theta^{SA1}$,
$^3J_{HnHn+1}$ – vicinal coupling constant [deg], ϕ – vicinal angle [deg], θ_{HnHn+1} – dihedral angle [deg].

Dihedral angles θ_{HnHn+1}1 [deg] can be calculated directly from vicinal angles ϕ [deg] with eq. 39-43, respectively from vicinal coupling constant $^3J_{HnHn+1}$ [Hz] (eq. 50, 51).

$$trans\ \phi = (^3J_{HH})^2 \qquad (59)$$

$$cis\ \phi = (2x^3J_{HH})^2 \qquad (60)$$

a. Calculation of the dihedral angle from vicinal angle:

$$cis,\ trans\text{-}ee: \sin^{-1}\cos\phi = \theta_{HnHn+1}, \qquad (61)$$

$$trans\text{-}aa: \cos^{-1}\sin(-\phi) = \theta_{HnHn+1}, \qquad (62)$$

$$cis,\ trans\text{-}ee: \tan^{-1}\sin(-\phi) = Y, \qquad (63)$$

$$cis,\ trans\text{-}ee: \tan^{-1}(1/\sin\text{-}\phi) = Y, \qquad (64)$$

$$cis,\ trans\text{-}ee: \sin^{-1}\tan(-\phi) = Y, \qquad (65)$$

Vicinal angles ϕ [deg], and no at list vicinal coupling constant $^3J_{HnHn+1}$ [Hz], can be calculated with eq. 66 - 73 from dihedral angles θ_{HnHn+1} [deg] calculated from chemical shift δ [ppm].

b. Calculation of the vicinal angle from dihedral angle:

$$cis,\ trans\text{-}ee: \sin^{-1}\cos\theta_{HnHn+1} = \phi \qquad (66)$$

$\phi < 90$ [deg]

$$trans\text{-}aa: -\cos^{-1}\sin\theta_{HnHn+1} = \phi \qquad (67)$$

$$cis,\ trans\text{-}ee: -\sin^{-1}\tan Y = \phi \qquad (68)$$

$$cis,\ trans\text{-}ee: -\tan^{-1}(1/\sin Y) = \phi \qquad (69)$$

$\phi > 90$ [deg]

$$trans\text{-}aa: 180 + \cos^{-1}\sin\theta_{HnHn+1} = \phi \qquad (70)$$

$$cis,\ trans\text{-}ee: 180 - \sin^{-1}\tan Y = \phi \qquad (71)$$

$$cis,\ trans\text{-}ee: 180 - \tan^{-1}(1/\sin Y) = \phi \qquad (72)$$

where: $Y = \theta_{HnHn+1}$ - dihedral angle or $\theta_{n,n+1}$ - torsional angle.

Calculation of the vicinal coupling constant from vicinal angle:

The equations 73, 74 for calculation of the vicinal coupling constant are used between 0 - 6.1 [Hz] for *cis* and *trans-ee* stereochemistry and between 5.5 – 13.4 [Hz] for *trans-aa* stereochemistry. A switch between eq. 60 and 61 is required when *cis*-$^3J_{HH}$ [Hz] has values characteristic for *trans* stereochemistry and *trans*-$^3J_{HH}$ [Hz] characteristic for *cis* stereochemistry.

$$trans\ ^3J_{HH} = (\phi)^{1/2} \qquad (73)$$

$$cis\ ^3J_{HH} = (\phi)^{1/2}/2 \qquad (74)$$

$$^3J_{HH} = (\phi + \cos^2\theta_{HnHn+1})^{1/2}/2 \qquad (75)$$

Hopf fibration and two angles on two sets angles:
Real Hopf fibration: $S^0 \rightarrow S^1 \rightarrow S1$:

$$X^0 = \cos\theta^A\sin\theta^B \qquad (76)$$

R^4: *Hopf fibration* $S^1 \to S^3 \to S^2$ in case of relationship between angles of two sets:

$$X_0 = \cos\theta^B \sin\theta^A, \; X_1 = \sin\theta^B \sin\theta^B \qquad (77)$$

$$X_2 = \cos\theta^A \sin\theta^B, \; X_3 = \sin\theta^A \sin\theta^A \qquad (78)$$

R^{16}: octonionic *Hopf fibration* $S^7 \to S^{15} \to S^8$, quaternionic multiplication $S^3 \to S^7 \to S^4$.

4. Conclusion

3-Sphere theory enable calculation of the vicinal coupling constants $^3J_{HnHn+1}$ [Hz] from NMR data, a wave approach, through the manifold (rectangle, Carnot's Theorem, Hopf fibration, conic section) with trigonometric and algebraic equations, using Conic section, Hopf fibration and Lie algebra.

The fibration of the torsional angles analyzed with Hückel 1 reveals real Hopf fibration for n 7, and the quaterionic group Sp(2), Sp(1)cSO(8), the Spin(9)cSO(16) for n 9, and octonionic Hopf fibration for n 15 with Hückel 1and Hückel 2.

Forth's angles, dihedral θ_{HnHn+1} [deg] – vicinal ϕ [deg] and tetrahedral φ_{Cn} [deg] – internal γ [deg] easy to calculate from NMR data, usefully for determination of the phase angle of the pseudorotation with VISION Molecular models. Configurational analysis at anomeric position with 3-sphere dihedral angles having known stereochemistry and sign became an advantage when the domain of the vicinal coupling constant is uncertain for *cis* and *trans* stereochemistry [28].

Bond distances $l_{CnCn+1}[A^0]$ of five membered ring [29] iminocyclitols 1, 2 are calculated from dihedral angles. All attempts to found relationship between dihedral angles – vicinal angles - tetrahedral angles – and bond distances on seven sets units now are replaced by the graph and homotopic approach, Table 1 giving the equations 17, 18 for calculation of bond distances.

Conflicts of Interest

The authors declare no conflicts of interest.

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