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Research Article

3-Spherical Conformational Insights into Iminocyclitols with 1-α-D-Ribose and 1-β-L-Ribose Stereochemistry Under Homotopic Behaviour of Nuclear Magnetic Resonance Data

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Abstract

3-Sphere, a hypersphere in 4 dimensions approach, applied for calculating stereochemical parameters of iminocyclitol 1 – 5 with Hopf fibration and Lie algebra is described. Three angles have been considered, *i.e.* dihedral θ_{HnHn+1} [deg] – tetrahedral φ_{Cn} [deg] – phase angle of the pseudorotation P [deg] calculated from NMR data, vicinal coupling constant $^3J_{HH}$ [Hz] and carbon chemical shift δ_C [ppm]. This approach gave for 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 2 two conformers E_3 and $^3T_2$ having different dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles with same vicinal angles ϕ [deg]. Notably, phase angle of pseudorotation P [deg] placed the conformations on the south side for D-ribitols 1 - 3 and on the north side for L-ribitol 4, excepting trifluoroacetate salt of L-ribitol 5. The wave character of NMR data introduced few homotopic switches, the transformation from torus to inverse of torus, the relationship between angles of set A and set B, the transformation from Planck constants h to h-bar, along with the transformation from Joule to Calorie (J 4.1868 ⇆ J^{-1} 0.238). Two methods for calculation of tetrahedral angles φ_{Cn} [deg], energy-graph and Euler conic with two ways for representing the angles, polyhedron and unit models are analyzed. The conformational parameters, phase angle of the pseudorotation P [deg] established with VISION molecular model and exocyclic 3-Sphere dihedral angles θ_{HnHn+1} [deg] relative to endocyclic torsional angles $\theta_{n,n+1}$ [deg] from Altona-Sundaralingan model have been evaluated. In addition, the corresponding angle of deviation from planarity θ_m [deg] has been determined.

Keyword

3-Sphere, Dihedral Angles, Vicinal Angles, Vicinal Coupling Constant, Tetrahedral Angles, Phase Angle of the Pseudorotation, Angle of Deviation from Planarity, Conformational Analysis, Iminocyclitols

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1. Introduction

3-Sphere dihedral angles θ_{HnHn+1} [deg] on five membered ring can be calculated from vicinal coupling constant $^3J_{HH}$ [Hz] and / or chemical shift δ [ppm] with Hopf fibration and Lie algebra protocol. [1] The Hopf fibration trigonometric model, in agreement with the algebraic equations, and the 3-Sphere representation of six dihedral angles with *cis-*, *trans-ee* and *trans-aa* stereochemistry ensure calculation of dihedral angles θ_{HnHn+1} [deg] with right sign and stereochemistry in close relationship with vicinal angle ϕ [deg]. The angles are placed on two units with three sets of angles (A, B, C), with two sets (A, B) per unit from the trigonometric point of view and considering the relationships between the vicinal ϕ [deg] and dihedral angles θ_{HnHn+1} [deg]. [1-3] In the case of tetrahedral angles in close relationship with dihedral angles, seven sets of angles on one unit are preferred. [1] Moreover, Altona-Sundaralingan model [4] used endocyclic torsional angles $\theta_{n,n+1}$ [deg] for conformational analysis: phase angle of pseudorotation P [deg] and angle of deviation from planarity θ_m [deg]. In addition, Karplus dihedral angles [5], calculated from vicinal coupling constant $^3J_{HH}$ [deg], can be transformed in endocyclic torsional angles with PSEUROT equations, [6] a program able to give the right sign and stereochemistry useful for simulation of phase angle of the pseudorotation P [deg] with Gausian09W. [7]

Essentially, the 3-Sphere dihedral angles calculated from carbon and / or proton chemical shift [8] can be used on conformational analysis using exocyclic angles [9] on Altona-Sundaralingan model [10]. By contrast, the phase angle of pseudorotation P [deg] can be evaluated with VISION molecular model [11]. In the present work, 3-Sphere approach was designed for establishing the relationship between different dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles with the same vicinal angle ϕ [deg] for iminocyclitols 1 – 5 [12] with equations (1-5).

$$P = \tan\text{-}1\ [(\theta 3,4 - \theta 1,2)/3.077 x \theta 2,3] \quad (1)$$

$$\theta m = \theta 2,3/\cos P \quad (2)$$

$\theta_{H2H3} < 0$:

$$P = -\ (180\ -\ Pcalc) \quad (3)$$

$$P = 180 + P^{calc} \quad (4)$$

Where P^{calc} [deg] – phase angle of the pseudoroation calculated with Altona-Sundaralingan Eq. (3) for P^{calc} positive and with eq. (3) for P^{calc} negative; $\theta_{n,n+1}$ [deg] – endocyclic torsional angle, used in Table 5 also as $\theta_{HnH,n+1}$ [deg] exocyclic torsional angle.

$$\theta_m = \theta_{2,3}/\cos P^{calc} \quad (5)$$

Where θ_m – angle of deviation from planarity [deg] calculated from P^{calc} for $\theta_{2,3} < 0$ [deg].

2. Results

The vicinal coupling constant $^3J_{HH}$ [Hz] under 3-Sphere trigonometric equations [1-3] gives three possible dihedral angles θ_{HnHn+1} [deg] for every stereochemistry [1], considering vicinal coupling constant for *cis*, *trans-ee* stereochemistry with smaller values and for *trans-aa* stereochemistry with higher values [13, 14].

As recently demonstrated, vicinal coupling constant $^3J_{HH}$ [Hz] can be higher for *cis*, *trans-ee* and smaller for *trans-aa* [2], thus the number of possible dihedral angles θ_{HnHn+1} [deg] increased to six. Conformational characterization of iminocyclitols 1 – 5 with 1-α-D-ribitol and 1-β-L-ribitol stereochemistry (Figure 1) [12] presented in this paper was based on the relationship between dihedral θ_{HnHn+1} [deg] – tetrahedral φ_{Cn} [deg] and phase angle of pseudorotation P [deg]. In case of 3-Sphere dihedral angles θ_{HnHn+1} [deg], as found from trigonometric equations, [1] *cis* and corresponding *trans-aa* stereochemistry are under 180 [deg] rule and *cis* and *trans-ee* stereochemistry under 120 [deg] rule, [15] with *trans-ee*^{3,2} stereochemistry moving between two units, the unit U and unit S in 2D [3]. For iminocyclitols 1 - 5 proposed for conformational analysis the rule for calculating dihedral angles from second vicinal angle ϕ [deg] [2] gives one more dihedral angle for vicinal coupling constant of 3.9, 5.4, 5.2 [Hz] with *cis* stereochemistry. Iminocyclitol 2, 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol was used extensively in this paper for conformational analysis, since the calculated 3-Sphere dihedral angles θ_{HnHn+1} [deg] are difficult to simulate on VISION molecular model.

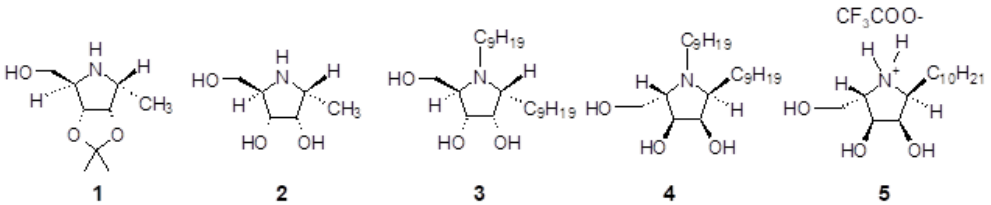

Figure 1. *Five membered ring iminocyclitols with α-D-ribitol (1-3) and β-L-ribitol (4, 5) stereochemistry.*

In this context, the dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles calculated from carbon chemical shifts [1, 16] for 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 2 [12] are chosen in pair of angles from seven sets units: *i. e.* dihedral θ_{HnHn+1} [deg] – vicinal ϕ [deg] from sets A and B and tetrahedral φ [deg] - internal γ [deg] from sets D, E or F, G, as presented in Table 1 without opposite rule and in Table 2 using opposite rule, dihedral from unit build with sin function and tetrahedral from unit build from tan function, or viceversa. Units are constructed from one angle of set A calculated from *sin* and *tan* function from carbon chemical shift δ_{Cn} [ppm] and Eular – conic manifold. [1] In function of the phase angle of the pseudorotation P [deg], dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles [16] are chosen from units in opposite mode for few possible conformers (Table 2). As an important remark, the transformations from U to S or S to U, two units with three sets angles ($C = U^{A,B,C}$, $S^{A,B,C}$), replace better two units with seven sets angles ($C = U^{A-G}$, S^{A-G}) calculated from *sin* and *tan* function. Between sets A and B one first angle must be higher than 5 [deg] on unit U and smaller than 5 [deg] on unit S. Building six sets in two units for compound 1 from C_2 carbon chemical shift δ_{C2} [ppm], it is obvious that the transformation from S to U can be made with angle on unit S of 6.85 [deg]. Alternatively, between six sets angles on two units, the equation is known [16] for calculation in opposite dihedral and tetrahedral angles from angle θ^{S4} of set A or B with equation (6). In case of iminocyclitol 1, from the unit build with C_3 under tan function with first angle of 7.05056 [deg] the transformation U to S gives the unit U instead of S, and the transformation S to U gives unit U. For the conformation of iminocyclitol 1 the NMR data in this case are somewhat difficult to be analyzed in strictly opposite rule.

$$\cos^{-1}\sin\{[60 - (\theta^{S4} - 90)]/1.5\} = \varphi_{Cn} \quad (6)$$

Where θ^{S4} [deg] – forth angle on set A or B of unit S, φ_{Cn} [deg] – tetrahedral angle of five membered ring.

The tetrahedral angles φ_{Cn} [deg] in relationship with the corresponding dihedral angles θ_{HnHn+1} [deg] are selected to be considered as well (Table 2). Two aspects are evident: 1. The dihedral θ_{HnHn+1} [deg] and tetrahedral angles φ_{Cn} [deg] are in opposite way on seven sets angles on unit U or S. That is also true on six sets angles on two units (U and S), or building more units U_2 or S_2 from U_1 or S_1; 2. Dihedral angles θ_{H3H4} for D-ribose stereochemistry with *trans-aa* vicinal coupling constant 8.8 [Hz] is over rule, dihedral and tetrahedral angles are found on sets D and E or F, G. In this case, for units S_1, the values calculated from sin and tan functions for vicinal coupling constant, are smaller (8.72, 8.71 [Hz]), but in S_2 both values increased to 8.79, 8.76 [Hz] almost equal with the recorded vicinal coupling constant $^3J_{H3H4}$ 8.8 [Hz].

In Table 3 the tetrahedral angles φ_{Cn} [deg] are calculated with energy-graph theory [17, 18] using Planck constant h and polyhedron equations (7-9) characteristic for icosahedron and dodecahedron, inversely of h giving h-bar with a factor of correction f 0.94767, and a transformation from Joule to Calorie (J 4.1868 ⇆ J^{-1} 0.238) under homotopic process [19]. Relative to building units, polyhedron model used first tetrahedral angle φ_{Cn} [deg] calculated from *sin* or *cos* functions on its relationship with corresponding internal angle γ [deg] under 180 [deg], and continuum transformation from internal γ [deg] (corresponding to θ^3) in tetrahedral φ [deg] (corresponding to θ^4) with polyhedron equation (7). In Table 4 are presented dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles [17, 18] calculated for E_3 and $^3T_2$ conformations with values comparable with angles [16] presented in Table 2.

$$\tan(A/2) = X = 2\sin^{-1}(B/2) \quad (7)$$

$$2x\tan^{-1}\{2x\sin[(180 - \theta)/2]\} = \varphi \sim 100 \text{ [deg]} \quad (8)$$

$$180 - \tan^{-1}(1/\{[(\sin[(180 - \theta)/2]\}/2) = \varphi \sim 106 \text{ [deg]} \quad (9)$$

Where θ ~ 105, 104 [deg].

Table 1. *Dihedral θ_{HnHn+1} [deg] [13, 14] and tetrahedral φ_{Cn} [deg] angles [16] of 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 2 [12] calculated from carbon chemical shift δ_{Cn} [ppm].*

Entry	$^3J_{HH}$ [Hz]	ϕ [deg]	δ_{Cn} [ppm]	ϕ [deg]	$^2J_{HH}$ [Hz]	θ_{HnHn+1}^{calc} [deg]	φ_{Cn}^{calc} [deg]
1.	*cis*: 3.1	38.44	C_1: 57.4	38.458	3.10	S: 51.541 T: -31.879	S – C_1: 109.229 S – C_2: 100.770 T – C_1: 105.770 T – C_2: 104.229
2.	*cis*: 3.9	60.84	C_2: 71.5	60.046	3.87	S: 29.953 T: -33.406	S – C_1: 105.023 S – C_2: 104.976 T – C_1: 106.733 T – C_2: 103.266
3.	trans-aa: 8.8	77.44	C_3: 71.7	60.138	3.87	S: 29.861 T: -33.530	S - C_4: 105.06 S - C_3: 104.93 T - C_4: 106.76

Entry	$^3J_{HH}$ [Hz]	ϕ [deg]	δ_{Cn} [ppm]	ϕ [deg]	$^2J_{HH}$ [Hz]	θ_{HnHn+1}^{calc} [deg]	φ_{Cn}^{calc} [deg]
4.			C_4: 66.8	76.152 75.939	8.72 8.71	S: -135.84[S1] T: -135.87[S1]	T - C_3: 103.23 S - C_4: 106.15 S - C_3: 103.84 T - C_4: 105.93 T - C_3: 104.06
				77.305 76.878	8.79 8.76	S: -135.708[S2] T: -135.75[S2]	S - C_4: 107.30 S - C_3: 102.69 T - C_4: 106.878 T - C_3: 103.121

a. D_2O δ [ppm] ^{13}C-NMR, 75 [MHz], ^{1}H – NMR 400 [MHz].

The phase angle of the pseudorotation P [deg] was established using exocyclic 3-Sphere dihedral angles on VISION molecular model [9] and Altona - Sundaralingam map [4]. In Table 5 the phase angles of pseudorotation P [deg] calculated with Altona Sundaralingan model [10] from exocyclic 3-Sphere dihedral angles [9] are presented in comparison with endocyclic torsional angles, and corresponding angles of deviation from planarity θ_m [deg]. Endocyclic torsional angles (eq. (10, 11)) calculated with method 2 [7] in function of trans or corresponding trans exocyclic dihedral angles and vicinal coupling constant (Table 6) gives on Altona – Sundaralingam equation (1) results comparable with conformation established on VISION molecular models.

$$\theta_{n,n+1} = \theta_{HnHn+1}{}^{trans\text{-}aa}/^3J_{HH} \quad (10)$$

$$\theta_{n,n+1} = (\theta_{HnHn+1}{}^{trans\text{-}ee} x\, ^3J_{HH})/2 \quad (11)$$

where $\theta_{n,n+1}$ torsional endocyclic angles [deg], θ_{HnHn+}1transexocyclic dihedral angles [deg].

3. Discussions

3.1. Conformational analysis: Phase Angle of the Pseudorotation P [deg], Angle of Deviation from Planarity θ_m [deg]

In the present study, the phase angles of the pseudorotation P [deg] are determined with VISION molecular models and 3-Sphere dihedral angles θ_{HnHn+1} [deg], exocyclic dihedral angles [9, 20] calculated in this case directly from carbon chemical shift δ_{Cn} [ppm] (Tables 2, 4) in comparation with phase angles of the pseudorotation calculated with Altona equation (1) from exocyclic torsional angles [9] and endocyclic torsional angles $\theta_{n,n+1}$ [deg] in case of iminocyclitol 2 (Table 5) and only from endocyclic torsional angles $\theta_{n,n+1}$ [deg] for iminocyclitols 1, 3 - 5 (Table 6).

Endocyclic torsional angles $\theta_{n,n+1}$ [deg] are calculated from 3-Sphere dihedral angles $\theta_{Hn,Hn+1}$ [deg] with *method 1*: under 180/120 rule for *cis* stereochemistry and 120 rule for *trans* stereochemistry, *method 2*: endocyclic torsional angles are calculated from 3-Sphere dihedral angles and vicinal coupling constant conform with equations reported to date [7]. In both cases, the sign in *D-ribitol series*: positive *trans-ee* endocyclic torsional angle relative to negative dihedral angle θ_{H3H4} [deg], and in *L-ribitol series*: negative *trans-ee* endocyclic torsional angle relative to positive dihedral angle θ_{H3H4} [deg], as reported recently based on Gaussian09W analysis [7] on iminocyclitol 2. Phase angle of pseudprotation P [deg] calculated with endocyclic torsional angles $\theta_{n,n+1}$ [deg] with methods 2 in case of iminocyclitol 1 is 15.28 [deg] with a conformation near to E^3 comparative to method 1 with 7.63 [deg] at border line between $_2T^3$ and E^3 (Table 5, entry 2). According to our first analysis, the phase angle of pseudorotation of -143.12 [deg] with $_3E - {}^4T_3$ conformation [9] results for the combination of dihedral angles: I. 50.20, 29.67, -168.6 [deg] calculated with modified Altona model (eq. (1)) from exocyclic torsional angles [13]. Because the first combination of angles is too hard to simulate on molecular models, Sundaralingam theory [21] with two atoms out of plane (^{32}E) was considered. With both positive angles for *cis* stereochemistry, the *trans-aa* H_3H_4 angle negative from D-ribitol stereochemistry becomes smaller as 90 [deg]. Subsequently, the optimized method for calculation of the dihedral angles from trigonometric equations [14] point out other two combinations: II. $_3E$ 50.20, -40.98, -135.57 [deg], III. $^3T_2$: -52.53, 29.67, -168.36 [deg]. [9] The opposite trigonometric relationship between dihedral and tetrahedral angles sin *versus* tan function for building units or vice *versa* reveals unexpected relationship between two combinations of angles (Table 2): I. 51.54, -33.46 or -33.53, -135.708 [deg]: S – T – T – S (Table 2, entry 1-4, Table 5, entry 1) and II. -31.87, 29.95 or 29.86, -135.757 [deg]: T – S – S – T (Table 2, entry 5 – 8, Table 5, entry 2), with E_3 (-162 [deg]) and E_2 (-18 [deg]) conformations analyzed with VISION molecular models, comparative to phase angle of pseudorotation P [deg] calculated with Altona-Sundaralingan eq. (1) from endocyclic 3-Sphere torsional angles: E_3 (-163.51 [deg], -153.8 [deg]) and $^3T_2$ - E^3 (7.63 [deg], 15.28 [deg]). In second case from exocyclic angles resulting a phase angle of the pseudorotation P [deg]

of -7.65 [deg] with a conformation between $E_2 - {}^3T_2$. On VISION molecular model conformation E_3 can be simulated with a good balance between angle of deviation from planarity θ_m [deg] and 3-Sphere dihedral angle θ_{H2H3} [deg] (Table 5, entry 1, 3 - 5), otherwise dihedral angles θ_{H3H4} with *trans-aa*[5,2] stereochemistry becomes smaller as 120 [deg], near to 90 [deg] characteristic for *trans-ee* stereochemistry with tendency to become ${}^0T_4$ conformation with P 72 [deg], behavior recorded also with Gaussian09W [7, 22]: S – S – S – T having ${}^0E$ (90 [deg]) conformation. In Table 5, entry 1, 3 - 5, exocyclic dihedral angles (+) *cis*-θ_{H1H2} – (-) *cis*-θ_{H2H3} – (-) *trans-aa*[5,2] θ_{H3H4} with E_3 configuration have θ_{H2H3} -33.46, -41.15, -15.75 [deg], and angle of deviation from planarity θ_m -27.67, -20.67, -44.85 [deg] increasing since dihedral angle θ_{H2H3} [deg] decreased. Phase angle of pseudorotation calculated from exocyclic dihedral angles are different with 13 – 26 [deg] relative to endocyclic torsional angles (Table 5, entry 1, 3), higher difference (52 [deg]) resulting from smaller exocyclic angle θ_{H2H4} [deg] (Table 5, entry 4).

Conformation $E_2 - {}^3T_2$ (P -18 - 0 [deg]) having exocyclic dihedral angles (-) *cis*-θ_{H1H2} – (+) *cis*-θ_{H2H3} – (-) *trans-aa*[5,2] θ_{H3H4} simulated on molecular models are comparable with twist ${}^3T_2$ conformation calculated with Altona-Sundaralingan eq. (1) from endocyclic torsional angles $\theta_{n,n+1}$ [deg], phase angle of pseudorotation P 7.63 [deg] and angle of deviation from planarity θ_m 30.31 [deg].

Isopropylidene protected (1) and unprotected (3 - 5) iminocyclitols [12] with α-D-ribose (1, 3) and β-L-ribose (4, 5) stereochemistry, bearing nonyl chain at C_1 and NH (3, 4) and trifloroacetate salt with decyl at C_1 (5), shown conformations as calculated with eq. (1) from endocyclic torsional angles $\theta_{n,n+1}$ [deg], in south side for α-D-ribose stereochemistry and north side for β-L-ribose stereochemistry, excepting for β-L-stereochemistry trifuoroacetate salt iminocyclitol 5 (Table 6). Protected iminocyclitol 1 with methyl group at C_1 and unprotected 3 with nonyl at C_1 and NH, have the following conformation: twist ${}^2T_3$ (-175.5, -173.9 [deg] 1), twist ${}^2T_3$ conformation (-168.021 [deg] 3) or envelope E_3 conformation (-163.46 [deg] 3), since iminocyclitol 2 shown two conformations from E^3 (15.28 [deg]) and ${}^4T_3 - E_3$ (-153.8 [deg]). Nonyl chain at C_1 and NH on iminocyclitols 3 and 4 with D and L-ribose stereochemistry having conformation ${}^2T_3$ (-168.021 [deg]) – E_3 (-163.46 [deg]) and ${}^3T_2 - E^3$ (11.91 [deg]) – ${}^3T_2$ (1.312 [deg]) between south to north side of the 2D map. Phase angle of pseudorotation of trifloroacetate salt (5) with decyl chain at C_1 is placed in south side with ${}^2T_3 - E_3$ conformation (-174.01 [deg]). Conformation simulated on VISION molecular models are compatible with angles calculated from endocyclic torsional angles $\theta_{n,n+1}$ [deg], excepting P 11.91 with dihedral angles -2.92, 19.83, 88.99 [deg] (4). In Table 6 are presented tetrahedral angles in opposite relationship with dihedral angles, sin versus tan function. Between D-ribose 3 and L-ribose 4 iminocyclitols the conformations are change from south to north because in case of 3 dihedral angles θ_{H1H2} negative and θ_{H2H3} positive on molecular models give for θ_{H3H4} *trans-aa* stereochemistry instead of *trans-ee*.

3.2. Homotopic Behavior of NMR Data

The wave character of NMR data introduces few homotopic switches on relationship between vicinal – dihedral – tetrahydric angles, at list on phase angle of the pseudorotation P [deg]. One topological space under continuous deformation *from one* to other [19], *i.e.* transformation from Planck constant h to h-bar, along with transformation from Joule to Calorie (J 4.1868 ⇆ J^{-1} 0.238), transformation from torus to invers of torus (sin *versus* tan functions), relationship between angles of set A and set B.

Relationships between *vicinal* ϕ – *dihedral* θ_{HnHn+1} – *tetrahedral* φ_{Cn} *angles* [deg] and at least *phase angle of pseudorotation* P [deg] are used for establishing the real combination between calculated dihedral angles θ_{HnHn+1} [deg] from only one recorded vicinal coupling constant ${}^3J_{HH}$ [Hz] with two possible vicinal angles ϕ [deg], [2] totally six dihedral angles θ_{HnHn+1} [deg]. Six dihedral angles are calculated for vicinal coupling constant higher as 4.5 [Hz], [2] in this case for 3.9 [Hz] from carbon chemical shift C_4 result an angle of -15.939 [deg] with a vicinal coupling constant of 3.92 [Hz] from second rule [2]. The sign of *trans-aa* θ_{H3H4} [deg] is restricted by D ribitol – stereochemistry, negative only from first rule [14], since from second rule [2] result only positive angles. The stereochemistry of D-ribitol iminocyclitol 1 was established based on the method of synthesis chosen [12] and confirmed by H-H COSY, H-C HMQC NMR experiments (ind. 16 Supporting information).

Having in mind the tetrahedral angles of natural crystal pyrite of 106.6, 102.6, 102.6, 106.6, 121.6 [deg], until now all the calculated tetrahedral angles φ_{Cn} [deg] are recalculated with golden angle and golden ratio (Table 3), as relationships between angles of polyhedron and its pentagon unit [17].

Moreover, the tetrahedral angles calculated Energy-graph approach [17] using inverse of h-Planck are almost equals with angles calculated with Euler-conic section (Tables 3 and 4 in comparation with Tables 1, 2) [16], polyhedron *versus* unit for angles representation. The relationships between tetrahedral φ_{Cn} [deg] and dihedral θ_{HnHn+1} [deg] angles as a function of phase angle of the pseudorotation P [deg] (Tables 1 and 2) shown for E_3 conformation smaller value for φ_{C1}, φ_{C4} tetrahedral angles (105.77, 105.93 [deg]) and higher for φ_{C2}, φ_{C3} tetrahedral angles (104.97 and 104.93 [deg]) (Table 4). In addition, for ${}^3T_2$ conformation (Table 5, entry 2) the value on first unit (109.22 [deg]) are equal with φ_{C1} tetrahedral angle calculated with polyhedron equation 109.8 [deg] [15] from inverse of square energy in J/molx10^{-6} (Table 4), relative to 106.91 [deg] (Tables 2, 3).

Notably, the conformation E_3 with the following succession of angles φ_{Cn} (θ_{HnHn+1}) [deg]: Euler conic 105.77 (51.54), 104.97 (-33.40), 104.93 (-33.53), 105.93 (-133.12) [deg] (Table 2) and Energy-graph 105.38 (50.39), 104.54 (-33.80), 104.18 (-33.71), 105.09 (-135.58) (Table 4), relatively hard to

simulate on molecular models, and with values of tetrahedral angles unexpected, but result directly from building unit in case of Euler conic approach (Tables 1, 2), are confirmed by the angles calculated with Energy-graph approach using inverse of h-bar and polynomial equations (Tables 3 and 4). Furthermore, the tetrahedral angles can be transformed in values near to 100 and 106 [deg] with polyhedron equations (7, 8) [16, 17] as follows: 105.77 (106.78), 104.97 (101.22), 104.93 (101.24), 105.93 (106.75) [deg] (Table 2), near to theoretical values of five membered ring.

Table 2. *Phase angle of the pseudorotation P [deg] established with VISION molecular models from dihedral θ_{HnHn+1} [deg] [2, 13, 14] and tetrahedral φ_{Cn} [deg] angles [16] of 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 2 [12] calculated from carbon chemical shift δ_{Cn} [ppm] and vicinal coupling constant $^3J_{HH}$ [Hz].*

Entry	C_n[a]	θ_{HnHn+1} [deg]	$^3J_{HH}$ [Hz]	φ_{Cn} [deg]	C_n[c] [deg]	$\varphi_{Cn}{}^{Td}$ [deg]	Entry	θ_{HnHn+1} [deg]	$^3J_{HH}$ [Hz]	φ_{Cn} [deg]	C_n [deg]	Entry	θ_{HnHn+1} [deg]	$^3J_{HH}$ [Hz]	φ_{Cn} [deg]
1.	C_1	S: 51.54	3.10	T: 105.77	109.48[c]	106.789	5.	T: -31.87	3.1	S: 109.22	106.91[c]	9.	S: 51.54	3.1	T: 105.77
2.	C_2	T: -33.46	3.91	S: 104.97	100.015	101.223	6.	S: 29.953	3.87	T: 103.266	101.155[c]	10.	StoU: 49.984	3.16	108.466[c], 110.57 or 99.42[e]
3.	C_3	T: -33.53	3.907	S: 104.93	101.040	101.249	7.	S: 29.861	3.87	T: 103.234	101.176[c]	11.	UtoS: -41.179 S: 29.86	3.90 3.87	100.040[c], 110.02 or 99.97[e] T: 103.23
4.	C_4[b]	S: ϕ 76.15[S1] -135.844 ϕ 77.30[S2] -135.708[S2]	8.72 8.79 [S2]	T: 105.93 [U1A]	S_2: 106.878	106.757	8.	T: ϕ 75.93[S1] -135.87[S1] ϕ 76.87[S1] -135.757[S2]	8.71 8.76	S: 106.15	S_2: 107.3	12.	T: ϕ 75.93[S1] -135.87[S1] ϕ 76.87[S2] -135.757[S2] T: -15.93[H3H2]	8.71 8.76 3.92	S: 106.15 S: 107.3, 111.34 or 98.65[f] S: 111.92 or 98.076[f]
5.		E_3						E_2 - $^3T_2$					E_3		

a. D_2O δ [ppm] ^{13}C-NMR, 75 MHz, ^{1}H – NMR 400 MHz, b. relationships between vicinal angle and tetrahedral angle, c. six sets on two units, d. $\varphi_{Cn}{}^T$ tetrahedral angles calculated from polynomial eq. (7-9), e. seven sets angles from unit U_1, f. seven sets angles on one unit from set D in case of S_1 and from set F in case of unit S_2.

Table 3. *Tetrahedral angles [17, 18] calculated from carbon chemical shift δ_{Cn} [ppm] in relationship with dihedral θ_{HnHn+1} [deg] and vicinal ϕ [deg] angles for iminocyclitol 2.*

Entry	δ_{Cn} [ppm][a]	1/E, θ [deg]	$1/E^{1/2}$, θ [deg]	$1/E^2$, θ [deg]	$^3J_{HH}$ [Hz], ϕ [deg], θ_{HnHn+1} [deg]
1.	C_1 57.4	0.58203	0.76291	0.338767	$1/E^2$: $^3J_{H1H2}$: 3.14 [Hz] $^3J_{H2H3} = \{[2x(109.80 - 90)]^{1/2}\}/2$ ϕ = 39.603 [deg] θ_{H1H2} = 50.396, -32.516 [deg]
		71.187	75.436	70.198	
		74.998	78.185	74.613	
		81.328	80.556	82.018	
		98.671	99.443	97.981	
		105.001	101.482	105.386	
		108.812	104.563	109.801	

Entry	δ_{Cn} [ppm][a]	1/E, θ [deg]	$1/E^{1/2}$, θ [deg]	$1/E^2$, θ [deg]	$^3J_{HH}$ [Hz], ϕ [deg], θ_{HnHn+1} [deg]
2.	C_2 71.5	116.826		117.139 → 116.664 108.308 108.116	$1/E^{1/2}$: $^3J_{H2H3}$: 3.90 [Hz] θ_{H2H3} = 2x(104.545 – 90) = 29.09 [deg] ϕ = 60.91deg] θ_{H2H3} 29.44, -33.804 [deg] $^3J_{H1H2}$: 3.13 [Hz] θ_{H1H2} = 2x(115.400 - 90) = 50.8 [deg] ϕ = 39.2 [deg]
		0.46725	0.68356	0.21833	
		68.573	72.367 76.632	77.389 64.778 75.963	
		73.975	80.523 75.454	77.356 72.464 76.823	
		83.183	86.246 78.505	77.304 86.055 78.185	
		96.816	99.476 101.494	102.643 93.944 101.814	
		106.624	93.753 103.367	102.695 107.535 103.176	
		111.427	104.545 104.545 (115.400)	102.611 115.222→104.036	
		117.638 ϕ = 62.361	107.632		
3.	C_3 71.7	1/E 0.46595	$1/E^{1/2}$ 0.68258	$1/E^2$ 0.217077	$1/E^{1/2}$: $^3J_{H2H3}$: 3.904 [Hz] θ_{H2H3} = 2x(104.515 – 90) = 29.03 [deg] ϕ = 60.97 [deg] θ_{H2H3} 29.03, -33.71 [deg]
		68.909	63.579 75.484	64.920 75.514	
		74.1083	72.443 76.643	72.521 76.973 76.654	
		79.3703	86.096 78.487	85.943 76.363 78.468	
		82.9385	93.903 101.512	94.056 77.934 101.531	
		97.0614	99.527 103.356	104.485 102.064 103.343	
		100.629	104.515→104.515, 115.390	107.471 103.020 104.485	
		105.8916	107.556	115.079 → 103.636	
		111.090	116.420		
4.	C_4 66.8	0.500134	0.707201	0.25013409	$1/E^{2:}$ $^3J_{H3H4}$= 8.85 [Hz] ϕ = 78.468 [deg] θ_{H3H4} = -168.22, -135.58 [deg] 1/E: $^3J_{H2H3}$ = 3.87 [Hz] ϕ = 60.017 [deg] θ_{H2H3} = 29.982deg]
			70.536	61.03	
		60.017	74.745	75.514 70.949	
		70.536	81.781	76.654 81.495	
		89.984	89.983	78.468 89.117	
		90.015	90.016	101.531 90.882	
		109.463	98.218	103.345 98.506	
		119.982	105.254	104.485 105.093	
			109.463	115.379 109.051	
				118.97 116.0, 106.46	
5.	NH 3.33	0.531585	0.729099	0.2825831	
		115.354	93.6218, 115.630	114.3422	
			111.117, 107.699	106.4122	

a. D_2O δ_{Cn} [ppm], ^1H NMR 400 [MHz], ^{13}C NMR 75 [MHz].

Table 4. *Phase angle of the pseudorotation P [deg] established with VISION molecular models from dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles [17, 18] of 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 2 [12] calculated from carbon chemical shift δ_{Cn} [ppm] and vicinal coupling constant $^3J_{HH}$ [Hz].*

Entry	C_φ[a]	θ_{HnHn+1} [deg]	$^3J_{HH}$ [Hz]	φ_{Cn} [deg]	φ_{Cn}^{Tb} [deg]	Entry	θ_{HnHn+1} [deg]	$^3J_{HH}$ [Hz]	φ_{Cn} [deg]
1.	C_1	$1/E^2$: 50.396	3.14	105.38	106.86	5.	$1/E^2$: -32.516	3.14	109.801 (108.11)
2.	C_2	$1/E^{1/2}$: -33.804	3.90	104.54	101.49	6.	$1/E^{1/2}$: 29.44	3.89	103.36 (101.49)
3.	C_3	$1/E^{1/2}$: -33.71	3.90	104.18	101.72	7.	$1/E^{1/2}$: 28.36	3.92	103.23 (101.72)
4.	C_4	$1/E^2$: -135.58	8.85	105.09	106.91	8.	$1/E^2$: -135.58	8.85	109.051 (106.46)
5.		E_3					E_2 - $^3T_2$		

a. D_2O.δ [ppm] ^{13}C-NMR, 75 MHz, ^{1}H – NMR 400 MHz, b. φ_{Cn}^T tetrahedral angles calculated from polyhedron equations (6-8).

Table 5. *Phase angle of the pseudorotation P [deg] and angle of deviation from planarity θ_m [deg] calculated with optimized Altona-Sundaralingan model (eq. (1-5)) for iminocyclitol 2.*

Entry	Vision	θ_{HnHn+1}[a] [deg]	P [deg]	θ_m [deg]	$\theta_{n,n+1}$[b] [deg] Met. 1	P [deg]	θ_m [deg]	$\theta_{n,n+1}$[b] [deg] Met. 2	P [deg]	θ_m [deg]
1.	~E_3	51.54 -33.46 -135.708	-137.052 $^4T_3$ – E^4	-45.711	8.46 -26.54 -15.708	-163.514 E_3	-27.677	41.43 -37.57 -15.421	-153.809 $^4T_3$ – E_3	-41.872
2.	^3E	-31.87 29.953 -135.75	-7.65 $^3T_2$ – E_2	30.222	-28.13 31.047 -15.757	7.634 $^3T_2$	31.313	-47.783 38.473 -15.426	15.287 ^3E	39.884
3.	E_3	49.984 -41.155 -135.757	-143.347 $^4T_3$	-51.298	10.16 -18.845 -15.757	-156.036 E_3	-20.677	41.94 -35.601 -15.426	-152.359 $^4T_3$ - E_3	-29.026
4.	E_3	49.984 -15.939 -135.757	-117.494 ^4E	-35.525	10.016 -44.061 -15.757	-169.236 E_3	-44.850	41.940 -42.066 -15.426	-155.975 $^4T_3$ - E_3	-46.056

a. exocyclic 3-Sphere dihedral angles under 180 r ule for trans-aa stereochemistry, b. endocyclic torsional angles under 120 rule. Met. 1: 180/120 rule, Met. 2: $\theta_{n,n+1} = f(\theta_{HnHn+1}, {}^3J_{HH})$ [7].

Table 6. *Phase angle of the pseudorotation P [deg] and angle of deviation from planarity θ_m [deg] calculated with optimized Altona-Sundaralingan model (eq. (1-5)) for iminocyclitol 1, 3-6.*

Entry	Comp.	$^3J_{HnHn+1}$[a] [Hz]	δ_{Cn} [deg]	θ_{HnHn+1} [deg]	φ_{Cn} [deg]	Vision	θ_{HnHn+1} [deg]	$\theta_{n,n+1}$[b] [deg] Met. 1	P [deg]	θ_m [deg]	θ_{HnHn+1} [deg]	$\theta_{n,n+1}$[b] [deg] Met. 2	P [deg]	θ_m [deg]
1.		4.1	55.8	20.224	106.305		20.224	39.775	P -		20.224	38.969	P -	
2.	1	5.4	83.5	-25.311 -34.688[b]	101.5744	$^2T_3$	-25.311 -88.447	-34.68 31.553	175.594 $^2T_3$	-41.720	-25.311 -88.447	-28.646 27.555	172.621 $^2T_3$	-28.885
3.		5.4	84.3	-25.051	101.474		20.224	39.775	P -	-25.452	20.224	38.969	P -	-25.431

Entry	Comp.	$^3J_{HnHn+1}$[a] [Hz]	δ_{Cn} [deg]	θ_{HnHn+1} [deg]	φ_{Cn} [deg]	Vision	θ_{HnHn+1} [deg]	$\theta_{n,n+1}$[b] [deg] Met. 1	P [deg]	θ_m [deg]	θ_{HnHn+1} [deg]	$\theta_{n,n+1}$[b] [deg] Met. 2	P [deg]	θ_m [deg]
4.		0	65.9	-34.946[b] -88.447	106.4007		-34.688 -88.447	-25.312 31.553	173.986 $^2T_3$		-34.688 -88.447	-25.312 27.551	173.973 $^2T_3$	
5.		4.8	63.7	-/+2.043 -25.913[b] 19.833	106.862 (105.36[c]) 101.261	$^2T_3$	2.043 -18.732 -88.992	57.95 -41.268 31.008	P -168.021 $^2T_3$- E_3	-42.186	2.043 -18.732 -88.992	37.074 -31.013 22.336	P -171.22 $^2T_3$	-31.380
6.	3	5.2	72.5	-30.500[b] -/+18.732 19.614	103.108 100.166 101.415									
7.		5.2	74.0	-31.155[b] -/+18.587	102.877 100.385	$^2T_3$	2.043 -30.5 -88.992	57.957 -29.5 31.008	P -163.464 E_3	-30.772	2.043 -30.5 -88.992	37.074 -28.75 22.3368	P -170.541 $^2T_3$	-29.146
8.		0	69.3	-88.992	106.372									
9.		4.8	68.4	-/+2.923[S2] -/+2.438[S1] -26.16[δC2]	107.438[S2] 106.796 (105.73[c]) 106.883 (105.250)[c]	$^3T_2$	-2.923 19.833 88.992	-57.077 40.167 -31.008	P 11.91 $^3T_2 – E^3$	41.050	-2.923 19.833 88.766	-36.891 30.801 -10.855	P 15.36 $^3T_2 – E^3$	31.942
10.	4	5.2	72.5	19.833 -30.500[b] -/+18.738	101.261 103.108 100.166									
11.		5.2	72.7	19.803 -30.589[b] -/+18.717	101.282 103.076 100.196	$^3T_2$	-26.16 19.833 88.992	-33.84 40.168 -31.008	P 1.312 $^3T_2$	40.178	-26.16 19.833 89.766	-32.05 30.801 -10.855	P 12.605 $^3T_2 – E^3$	31.562
12.		0	70.9	89.766	106.636									
13.		2.8	63.3	59.422	107.165									
14.		3.6	72.1	-13.171	104.839		59.422	0.578	P -174.017 $^2T_3$ - E_3	-47.289	59.422	43.063	P -169.043 $^2T_3$ - E_3	-47.289
15.	5	3.6	73.4	-12.968	104.558	E_3	-12.968	-47.032			-12.968	-46.397		
16.		8.8	63.9	166.98 135.745[d]	106.855 (105.404[c])		135.745	15.745			135.745	15.425		

a. δ_{Cn} [ppm] 1, 3 - 5: $CDCl_3$, ^1H NMR 400 [MHz], ^{13}C NMR 75 [MHz], b. second rule [2]; c. polyhedron equations (6-8), d. angle calculated from ϕ [deg]. Met. 1: 180/120 rule, Met. 2: $\theta_{n,n+1} = f(\theta_{HnHn+1}, {}^3J_{HH})$ [7].

Angles calculated from polynomial equation (6) are comparable with angles fund by building units or transformation from U to S or S to U; *i.e.* 106.91, 101.15, 101.17, 106.87 [deg] (Table 2).

Tetrahedral angles calculated from carbon C_1 chemical shifts with eq. (8) of 106.78 [deg] are almost equal with the angle 106.917 [deg] calculated on unit U_2 from sin function. In case of C_2 and C_3 on unit U_2 results angles in opposite 100.01 or 100.04 [deg], relative to polynomial angles calculated with eq. (7) of 101.223 and 101.249 [deg], closed to angles results directly 101.15, 101, 17 [deg]. Fibonacci numbers F^n, golden ratio φ and golden triangle giving angles of 103.6545 [deg] and 101.01 [deg] for tetrahedral angle (eq. (12-15)). [18]

$$F^n = \varphi^n - \Psi^n/(5)^{1/2} \quad (12)$$

Where: φ = 1.6180339887 goden ratio, Ψ =-1/φ = -0.6180339887 invers of golden ratio.

$$\gamma/2 = \cos^{-1}(\varphi/2) = \pi/5 = 36 \text{ [deg]} \quad (13)$$

$$2x\cos^{-1}(1/\varphi) = 103.6545 \text{ [deg]} \quad (14)$$

$$\varphi/2 = \cos^{-1}[(\varphi)^{1/2}/2) = 50.50 \text{ [deg]} \quad (15)$$

Where: γ – internal angle [deg], φ tetrahedral angle [deg].

4. Conclusions

Conformational parameter, phase angle of the pseudorotation P [deg] established with 3-Sphere approach gives for 1-α-methyl-1,4-imino-1,4-dideoxy-D-ribitol 1 two conformers E_3 and $^3T_2$ having different dihedral θ_{HnHn+1} [deg] and tetrahedral φ_{Cn} [deg] angles but same vicinal angles ϕ [deg]. From units are choose dihedral angles θ_{HnHn+1} [deg] with values of the corresponding vicinal angles ϕ [deg] almost equals with recorded. The alternation of the trigonometric functions corresponding to the first set of units is remarkable for the phase angle of pseudorotation, $^3T_2 – E_2$: N (7.4 [deg]), T-S-S-T (conform with VISION molecular models instead of endocyclic model) and E_3: S (-163 [deg]), S-T-T-S (Table 2). Considerable differences on phase angle of the pseudorotation (Table 5) are calculated from exocyclic torsional angles *cis*-$\theta_{Hn,Hn+1}$ [deg] [9] relative to endocyclic torsional angles $\theta_{n,n+1}$ [deg] calculated from 3-Sphere dihedral angles, in last case resulting a good correlation with conformations simulated on VISION molecular models. Conformations of D-ribose stereochemistry 1 and 3 are placed on south side, twist $^2T_3$ (1: -175.5, -173.9 [deg]), twist $^2T_3$ conformation (3: -168.021 [deg]) or envelope E_3 conformation (3: -163.46 [deg]) relative to L-ribose 4 in north side ($^3T_2 – E^3$ (11.91 [deg]) – $^3T_2$ (1.312 [deg])), excepting trifloroacetate salt with L-ribose stereochemistry 5 ($^2T_3 – E_3$ conformation (-174.01 [deg])). The angle of deviation from planarity θ_m [deg] decreased once the 3-Sphere dihedral angle θ_{H2H3} [deg] increased.

Noteworthy, endocyclic torsional angles $\theta_{n,n+1}$ [deg] are calculated from 3-Sphere dihedral angles $\theta_{Hn,Hn+1}$ [deg] with right sign selectively in function of the stereochemistry, D-ribitol *versus* L-ribitol and *trans-aa versus trans-ee*. Overall, homotopy approach on Planck constant was analyzed on relationship between dihedral θ_{HnHn+1} [deg] – tetrahedral φ_{Cn} [deg] angles, with losing 0.94767 at transformation from Planck h to Planck h-bar constants, in case of energy-graph approach (Tables 3, 4) as compared to Euler-conic approach (Tables 1, 2), two ways for transforming carbon chemical shift from ppm to J/molx10^6 or Gauss with polyhedron model (Table 3) or unit (Table 2). Also, two ways to establish the relationships between dihedral $\theta_{Hn,Hn+1}$ [deg] and tetrahedral φ_{Cn} [deg] angles, in function of the phase angle of the pseudorotation P [deg], were consistently employed.

Abbreviations

RMN Data Nuclear Magnetic Resonance Data

Conflicts of Interest

The authors have not conflict of interest.

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