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Research Article

Conic Projection as Manifold and 3-Sphere Dihedral Angles θ_{HnHn+1}[Deg] Under Homotopy

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Abstract

Conic projection as manifold enable calculation dihedral θ_{HnHn+1}[deg] angles from differences between two atoms of carbon $\Delta\delta_{CnCn+1}$[ppm] in three steps or from only one atom of carbon δ_{Cn}[ppm] in close relationships with tetrahedral φ_{Cn}[deg] angles under 3-Sphere approach. Hopf fibration and Lie algebra ensuring calculation dihedral θ_{HnHn+1}[deg] angles from vicinal ϕ[deg] angle, angle results from vicinal coupling constant $^3J_{HH}$[Hz]. Real Hopf fibration for calculation dihedral θ_{HnHn+1}[deg] angle in real space, and R^{16} octonionic Hopf fibration, double of quaternionic R^7, for all *cis*, *trans-ee*, *trans-aa* stereochemistry, unreal space relative to calculated dihedral θ_{HnHn+1}[deg] angle. Continue "deformation", homotopic behaviour h ⇆ h^{-1} characteristic for wave NMR data, probably a point of swich on Möbius band, in case of radius r of the cone inscribes on sphere at tangent point, calculated from height of cone h or inverse of height h^{-1}, the tan function of h is equal with sin function of h^{-1}. Dihedral θ_{HnHn+1}[deg] and tetrahedral φ_{Cn}[deg] angles are from the trigonometric point of view under sin and tan function, or *viceversa*, homotopic behavior of NMR data under conic projection demonstrating that. Because the dihedral θ_{HnHn+1}[deg] angles are not found in first unit, for few vicinal coupling constants $^3J_{HH}$[Hz], the rule accepted until now are explored taking in consideration other sets for building unit along the set C, respectively D, E and F, G, or vicinal angle ϕ[deg] with its three possible dihedral θ_{HnHn+1}[deg] angles in close relationships with tetrahedral φ_{Cn}[deg] angles under seven sets unit. Building units through sets U or S calculated from *sin* or *tan* functions until calculated angles are almost equals with angles of unit U_1 or S_1, required long time for calculation.

Keywords

Conic Projection, Homotopy, 3-Sphere Dihedral Angles, Tetrahedral Angles, Vicinal Coupling Constant

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1. Introduction

The invers of any closed curve on S^2 will be an immersed torus in S^3, and any compact Rieman surface of genus 1 can be embedded in the unit sphere S^3CR^4 as a flat torus. The embedding can be chosen as the intersecting of S^3 with a quadric hypersurface in R^4 [1]. As claimed by Willmore Conjecture surface in R^3 rather as S^3. [2] Surface in 3D Euclidean space R^3 is study with Möbius differential geometry, [2] measurement of angles instead of lengths, *i.e.* Plank-Einstein *versus* De Broglie [3, 4].

Conic projection used on spherical map calculation (*i.e.* earth map), convert the latitude and longitude coordinates into two-dimensional coordinate, cartesian coordinate. Point of sphere or spheroid are transformed in tangent or secant of cone that is wrapped around the sphere (Figure 1, eq. (1)-(3)) [5].

$$\theta = \sec^{-1}h \quad (1)$$

$$r = (h^2 - 1)^{1/2}/h \quad (2)$$

$$z = \cos\theta = 1/h \quad (3)$$

Where: h – height [radieni], r – radius of cone inscribes on sphere at tangent or secant point of the cone outside of sphere [radieni].

Six dihedral angles with *cis*, *trans*-aa, *trans-ee* stereochemistry can be represented on three concentric cons in 3D and on two intersecting circles in 2D. Point of intersection in 2D between two circles are half ϕ_1^A and ϕ_1^B, first angles of sets A and B or half angles $\phi_1^{A \text{ or } B}/2$ between *trans-ee*^{3,2} and *trans-ee*^{4,1}. Inside of the 3-Sphere, a hypersphere in 4D, are easy to drawn three sets angles, third set intersecting sets A and B at half first C angle, angle used for increased number of units [6].

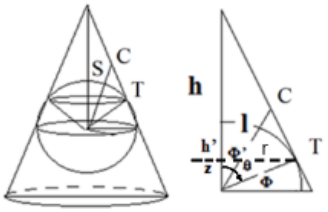

Figure 1. *Conic section representation.*

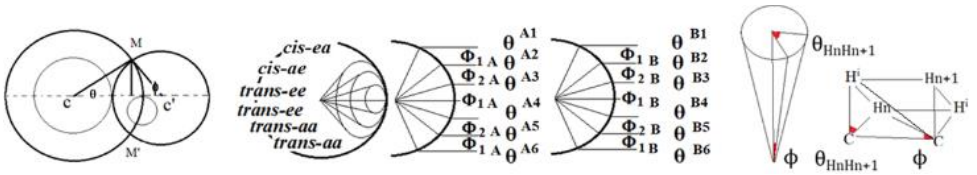

Figure 2. *Dihedral and vicinal angles on 3-Sphere representation.*

2. Results

Dihedral angles are calculated with conic projection (Figure 1) from differences between two atoms of carbon [7] or one atom of carbon in 3 steps as presented in Tables 1, 2 for iminocyclitols 1 - 8 (Figure 3) [8, 9]. The wave character of NMR data preserved homotopy, and angles calculated are under height h or invers of height h^{-1} since the calculated vicinal angle must be almost equal with the recorded one or with very smaller differences. The *tan* function of h^{-1} is equal with *sin* function of h ensuring the trigonometric rule between dihedral θ_{HnHn+1}[deg] and tetrahedral φ_{Cn}[deg] angles of five membered ring [10] (Table 2).

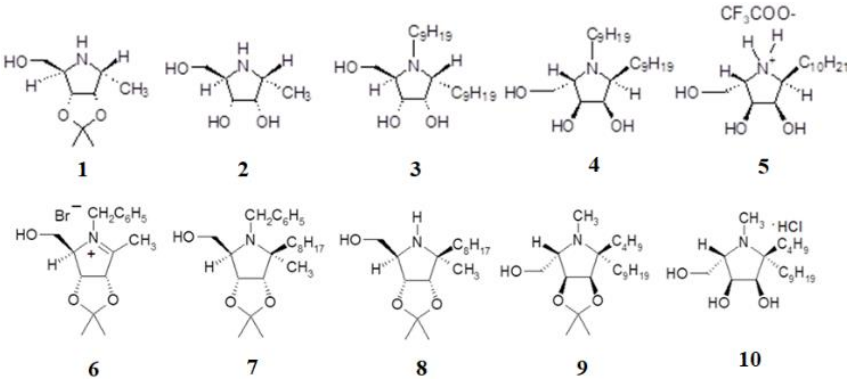

Figure 3. *Iminocyclitols with 1-α-D (1 – 3, 6 - 8) and 1-β-L-stereochemistry (4, 5, 9, 10) bearing at C_1 one alkyl chain or two alkyl chain.*

2.1. Method for Calculation Dihedral Angles in Three Steps

Step 1: Height of cone outside of sphere (eq. (5)) will be calculated from differences between two atoms of carbon $\Delta\delta_{CnCn+1}$[ppm] under Euler conic manifold (eq. (4)). The angle θ^{AIn} [deg] calculated with cos function from differences between two consecutive atoms of carbon chemical shift is transformed on first angle of the set A and calculate height of cone.

$$\cos^{-1}R_m = \theta^{Ain} \quad (4)$$

Where $\theta^{AIn} \rightarrow \theta^{AI1}$, n = 1 – 6.

$$\cos\theta^{AI1} = 1/h \quad (5)$$

Table 1. *Dihedral angles θ_{HnHn+1}[deg] calculated from differences between two atoms of carbons chemical shift $\Delta\delta_{CnCn+1}$[ppm] with conic projection for iminocyclitols 1-9.*

Comp	$^3J_{HH}$[a] [Hz]	Φ [deg]	$\Delta\delta_{CnCn+1}$ [gaussx10]	θ^{Ain} [deg]	θ^{AI1} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	ϕ [deg]	$^3J_{HnHn+1}$ [deg]	θ_{HnHn+1} [deg]
	4.1	67.24	0.755	39.11	20.88[b]	h^{-1}: 0.934	0.381	22.43	67.56	4.109	22.43
		16.81				h: 1.0703	0.356	20.88[b]	69.11[b]	4.15	20.88
		116.64	0.022	88.71	28.71	h^{-1}: 0.877	0.547	33.219	116.78	5.40	-26.78
		29.1									-41.756
											30.312
1	5.4								119.363	5.46	-41.073[c]
									28.715	5.35	-33.219
						1.1402	0.4804	28.715	118.715	5.44	-28.715
									118.420	5.44	-40.428[c]
	0		0.515	58.97	1.024	0.999	0.0178	1.0247	1.02471	0.5060.	-88.97, -91.024
						1.0001	0.0178	1.0246	0246	506	-88.97, -91.024
		38.44	0.3949	66.736	6.7366	0.993	0.1181	6.7837	38.69	3.11	-53.216
		9.61							40.24	3.17	-32.861[S3]
									9.648	3.106	-9.514[d, US]
									9.648	3.106	-9.788[d, US]
	3.1								39.648	3.14	50.351[US]
						1.0069	0.1173	6.7366	38.691	3.11	-53.263
									9.790	3.12	-9.936
									9.70	3.12	-9.936
2									39.790	3.15	50.209
		60.84	0.0056	89.679	29.679	0.8688	0.5699	34.743	60.320	3.88	-34.743
		15.21							62.530	3.95	-41.581
	3.9					1.1509	0.4951	29.679	60.320	3.88	29.679
									62.617	3.95	-40.106
									15.160	3.89	-14.655[e]
	8.8	77.44	0.1372	82.110	22.110	0.9264	0.4062	23.971	78.014	8.82	-167.74, -135.63
		309.76				1.07938	0.3764	22.110	78.944	8.88	-168.73,

Comp	$^3J_{HH}$[a] [Hz]	Φ [deg]	$\Delta\delta_{CnCn+1}$ [gaussx10]	θ^{Ain} [deg]	θ^{AI1} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	ϕ [deg]	$^3J_{HnHn+1}$ [deg]	θ_{HnHn+1} [deg]
											-135.53
	4.8	92.16	0.24649	75.729	15.729	0.9625	0.2816	16.358	92.716	4.814	-/+2.716[S2]
		23.04				1.0389	0.2710	15.729	92.918	4.8519	-/+2.918[S3]
		108.16	0.0420	87.591	27.591	0.886	0.5226	31.507	108.457	5.207	19.497
	5.2	27.04							27.591	5.25	-31.507
3						1.1283	0.4631	27.591	28.188	5.30	-32.408
			0.13165	82.434	22.434	0.9243	0.4128	24.386	2.8069	0.83	-87.193
	0								1.4034	0.601	-88.596
						1.08188	0.3816	22.434	1.8913	0.687	-88.108
	4.8	92.16	0.07563	85.662	25.662	0.9013	0.4804	28.715	92.568	4.81	-/+2.568
		23.04				1.10943	0.4330	25.662	92.168	4.8	-/+2.168
		108.16	0.04481	87.431	27.431	0.8875	0.5190	31.268	27.431	5.23	-31.268
		27.04							108.524	5.20	-19.577
4	5.2					1.12667	0.4606	27.431	27.442	5.23	-31.284
									108.520	5.20	-19.571
			0.05042	87.109	27.109	0.8901	0.5119	30.793	0.793	0.44	-89.206
	0					1.12342	0.4556	27.109	1.445	0.60	-88.554
		31.36	0.24649	75.729	15.729	0.9625	0.2816	16.358	31.048	2.78	-27.283
		7.84							8.09709	2.84	-8.1791
	2.8					1.03890	0.2710	15.729	31.459	2.80	58.545
										2.8	-37.135
										2.8	-27.556
									7.7917	2.79	-7.8647
		51.84	0.03641	87.913	27.913	0.8836	0.5297	31.989	51.3264	3.582	38.6736
		12.96									-37.9798
5											-53.1678
	3.6					1.13165	0.4681	27.913	51.3912	3.584	38.6087
											-38.0049
											-52.9908
		77.44	0.26610	74.567	14.567	0.9678	0.2598	15.062	322.46	8.97	142.468
		309.76							79.958	8.94	169.958
	8.8					1.03321	0.2515	14.567	310.417	8.8	142.716
									79.711	8.92	168.711
		96.04	0.19607	78.692	18.692	0.94725	0.3383	19.775	24.887	4.98	-22.823, -27.640
6	4.9	24.01				1.05568	0.3294	18.692	24.618	4.96	-22.615
									24.346	4.93	-22.403, -26.903

Comp	$^3J_{HH}$[a] [Hz]	Φ [deg]	$\Delta\delta_{CnCn+1}$ [gaussx10]	θ^{Ain} [deg]	θ^{AIi} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	ϕ [deg]	$^3J_{HnHn+1}$ [deg]	θ_{HnHn+1} [deg]
7	0[a]		0.21848	77.379	17.379	0.95434	0.3129	18.239	2.64	0.812	-87.35
						1.04783	0.2987	17.379	3.93	0.99	-86.06
	7.6	231.04	0.10364	84.051	24.051	0.9131	0.4462	26.506	230.54	7.59	37.67
		57.76				1.0950	0.4075	24.051	58.253	7.63	31.746
									58.253	7.63	-40.377
									58.253	7.63	-38.224
		57.76	0.29971	72.559	12.559	0.9760	0.2120	12.242	58.061	3.809	-38.563
									58.031	3.808	-38.616
									57.872	3.80	32.128
											-40.259
	3.8										-38.901
		14.44				1.0245	0.2174	12.559	58.565	3.79	-37.677
									57.559	3.79	32.440
											-40.162
											-39.465
8	6.6	174.24	0.10364	84.051	24.051	0.9131	0.4462	26.506	43.253	6.57	46.746
		43.56				1.09507	0.4075	24.051	174.018	6.57	-/+5.948
	3.5	49	0.29971	72.559	12.559	0.9760	0.2227	12.864	12.5517	3.54	-12.864
		12.25				1.02451	0.2174	12.559	12.2679	3.50	-12.559
9	7.3	213.16	0.112	83.56	23.56	0.916	0.436	25.86	214.13	7.31	-55.87, -42.67, 29.29
		53.29							212.29	7.28	-57.93, -38.78, 27.96
						1.090	0.399	23.566	53.566	7.31	36.433, -38.81, -47.57
									213.217	7.30	-56.78, 28.71, -40.90
	4.5	20.25	0.3417	70.01	10.01	0.984	0.176	10.17	20.34	4.51	69.65
		81							80.34	4.49	170.34
						1.0158	0.173	10.01	20.008	4.47	69.99
									80.008	4.47	170.01

a.^{1}H, ^{13}C-NMR data ind. 8, 9; b. $\theta(r(h))^{sin} = \theta(r(h^{-1})^{tan}$; c. six sets; d. U to S giving U; e. from set D ; d polyhedron; e.U to S giving U.

Table 2. *Dihedral angles calculated θ_{HnHn+1}[deg] from carbon chemical shift δ_{Cn}[ppm] with conic projection for iminocyclitols 1-10.*

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AIi} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn}+1 [deg]	φ_{Cn} [deg]
1	4.1	67.24	C_1: 55.8	1.56302	50.224	9.775	0.9854	0.1722	9.9921	69.921	4.18	20.0787	109.88

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AIl} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn+1} [deg]	φ_{Cn} [deg]
		16.81					1.0147	0.1697	9.7757	69.775	4.17	20.2242	109.96
			C_2: 83.5	2.33893	64.688	4.688	0.9966	0.0820	4.7039	117.52	5.42	-41.567	99.218, 101.563[c]
										115.29	5.36	-25.296	102.655, 101.56[b]
										29.654	5.44	-34.703	102.655, 101.56[b]
							1.0033	0.0817	4.6895	117.53	5.42	-41.563	99.216, 101.567[c]
										115.31	5.369	-25.310	102.663, 101.565[b]
										29.645	5.44	-34.689	102.663, 101.565[b]
		116.6	C_3: 84.3	2.36694	65.008	5.008	0.9961	0.0876	5.0276	117.10	5.41	-41.675	99.162, 101.669[c]
		29.16								114.97	5.36	-24.972	102.495, 101.669[b]
	5.4									29.854	5.46	-35.027	102.495, 101.669[b]
							1.0038	0.0873	5.0084	117.12	5.41	-41.669	99.16, 101.675[c]
										114.99	5.36	-24.991	102.48, 101.67[b]
										29.842	5.46	-35.008	102.48, 101.67[b]
	0		C_4: 65.9	1.84593	57.198	2.801	0.9988	0.0489	2.8048	2.8048	0.837	-87.195	106.39
							1.0011	0.0488	2.8014	2.8014	0.836	-87.198	106.40
		38.44	C_1: 57.4	1.60784	51.541	8.458	0.9891	0.1487	8.5524	38.552	3.104	51.447	109.229, 106.917[b]
	3.1	9.61					1.0109	0.1470	8.4587	38.458	3.1	51.541	109.276, 107.104[b]
			C_2: 71.5	2.00280	60.046	0.046	0.9999	0.0008	0.0462	60.046	3.874	29.953	104.97, 100.015[b]
							1.0000	0.0008	0.0462	60.046	3.874	29.953	104.976, 100.015[b]
2		60.84	C_3: 71.7	2.00840	60.138	0.138	0.9999	0.0024	0.1383	60.138	3.877	29.861	104.93, 100.061[b]
	3.9	15.21					1.0000	0.0024	0.1383	60.132	3.877	29.861	104.93, 100.046[b]
		77.44	C_4: 66.8	1.87114	57.694	2.305	0.9991	0.0402	2.3081	76.154	8.72	-165.73	105.729[c]
		309.7								79.230	8.90	-169.03	109.036
	8.8									76.923	8.77	-166.56	106.571[U2,c]
										76.923	8.77	-135.75	105.752[d]

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AIl} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn}+1 [deg]	φ_{Cn} [deg]
							1.0008	0.0402	2.3053	76.152	8.72	-165.72	105.731[c]
										79.231	8.9	-169.03	109.035
										76.926	8.77	-166.57	106.568[U2,c]
										76.926	8.77	-135.75	105.752
		92.16	C_1: 63.7	1.78431	55.913	4.086	0.9974	0.0714	4.0966	23.598	4.85	-25.903	107.043
		23.04								92.048	4.79	+/-2.04[e]	106.02
							1.0025	0.0712	4.0862	23.606	4.85	-25.913	107.048
										92.043	4.796	+/-2.04[e]	106.021
	4.8		C_2: 72.5	2.03081	60.500	0.500	0.9999	0.0087	0.5006	26.909	5.187	-30.500	104.749, 100.166[b]
										109.83	5.21	19.833	99.916
							1.0000	0.0087	0.5006	26.909	5.18	-30.500	104.749, 100.166[b]
3										108.74	5.21	19.833	99.916
		108.1	C_3: 74.0	2.06511	61.037	1.037	0.9998	0.0181	1.0378	27.275	5.22	-31.037	104.481, 100.345[b]
		27.04								108.58	5.21	19.654	99.827
	5.2						1.0001	0.0181	1.0376	27.275	5.22	-31.037	104.481, 100.345[b]
										108.58	5.21	19.654	99.827
							0.9998	0.0175	1.0077	1.00771	0.501	-88.992	105.503, 109.664[b]1
	0		C_4: 69.3	1.94117	58.992	1.007	41.000	80.017	41.007	.0075	0.501	-88.992	05.502, 109.664[b]
		92.16	C_1: 68.4	1.91596	58.538	1.461	0.9996	0.0255	1.4622	92.924	4.81	-/+2.92	106.461
		23.04								22.541	4.74	-20.97	109.512
							1.0003	0.0255	1.4617	92.923	4.81	-/+2.92	106.462
										22.541	4.74	-20.974	109.512
	4.8		C_2: 71.1	1.99159	59.860	0.139	0.9999	0.0024	0.1396	26.661	5.163	-30.139	104.930
										108.84	5.216	19.953	110.023
							1.0000	0.0024	0.1396	26.661	5.163	-30.139	104.930
4										108.84	5.213	19.953	110.023
		108.1	C_3: 72.7	2.03641	60.589	0.589	0.9999	0.0102	0.5898	26.971	5.193	-30.589	104.705
		27.04								108.71	5.217	19.8033	110.098
	5.2						1.0000	0.0102	0.5897	26.970	5.193	-30.589	104.705
										108.71	5.213	19.803	110.098
			C_4: 70.9	1.98599	59.766	0.233	0.9999	0.0020	0.1167	0.1167	0.178	89.883	105.116
	0						1.0000	0.0040	0.2335	0.233	0.241	89.766	105.058
		31.36	C_1: 63.3	1.7731	55.668	4.331	0.9971	0.0757	4.3439	31.101	2.78	-37.104	109.33
5	2.8	7.84								7.1593	2.65	-7.104	109.33

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AIl} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn+1} [deg]	φ_{Cn} [deg]
										32.008	2.82	-38.687	108.556
							1.0028	0.0755	4.3315	31.105	2.78	-37.112	108.552
										7.167	2.67	-7.112	108.552
										31.994	2.828	-38.663	109.343
			C_2: 72.1	2.01960	60.320	0.320	0.9999	0.0055	0.3206	50.213	3.54	39.789	100.106
												-37.539	101.229[d]
												-56.383	103.191[d]
							1.0000	0.0055	0.3206	50.213	3.54	39.786	100.106
												-37.540	101.230[d]
												-56.383	103.191[d]
		51.84	C_3: 73.4	2.0560	60.897	0.897	0.9998	0.0156	0.8974	50.598	3.55	39.401	100.2
		12.96										-37.693	101.153[d]
												-55.276	102.615[d]
	3.6						1.0001	0.0156	0.8974	50.598	3.55	39.401	100.299
												-37.693	101.153[d]
												-55.231	102.638[d]
		77.44	C4: 63.9	1.7899	56.035	3.964	0.9976	0.0693	3.9744	76.987	8.77	166.987	106.98[c]
	8.8	309.7					1.0023	0.0691	3.9649	76.982	8.77	166.982	106.98[c]
		96.04	C_2: 78.4	2.19607	62.912	2.912	0.9987	0.0496	2.8471	24.530	4.95	-27.152	103.543
		24.01								95.694	4.89	-5.694[S2]	102.687
										95.666	4.89	5.694[S2]	102.687
										23.700	4.86	-21.89[U2]	100.970
							1.0012	0.0508	2.9120	95.824	4.89	-5.824[S2]	102.152
	4.9									95.794	4.89	5.824[S2]	102.152
6										23.755	4.87	-21.94[U2]	100.949
			C_3: 85.4	2.39215	65.289	5.289	0.9957	0.0925	5.3122	95.312	4.88	-5.312	102.355
										95.289	4.88	5.3122	102.355
							1.0042	0.0921	5.2895	95.289	4.88	-5.289	102.343
										95.267	4.88	5.289	102.343
							0.9989	0.0455	2.6122	2.61222	0.808	-87.38	106.30410
	0[a]		C_4: 77.6	2.1736	62.609	2.609	61.001	70.045	2.6095	.6095	0.807	-87.39	6.306
		231.0	C_2: 84.2	2.35854	64.913	4.913	0.9963	0.0859	4.9313	230.65	7.59	-55.068	102.543, 101.637[b]
		57.76								57.342	7.57	-39.862	100.086
7	7.6						1.0036	0.0856	4.9132	230.64	7.59	-55.086	102.534, 101.643[b]
										57.361	7.57	-39.826	100.068
			C_3: 80.5	2.25490	63.673	3.673	0.9979	0.0642	3.6815	230.23	7.58	-56.318	103.163,

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AIl} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn+1} [deg]	φ_{Cn} [deg]
													101.224[b]
										229.77	7.57	37.363	101.326
							1.0020	0.0640	3.6739	230.23	7.58	-56.326	103.159, 101.227[b]
										229.73	7.57	37.347	101.318
		57.76	C_4: 69.8	1.95518	58.238	0.761	0.9999	0.0138	0.7612	57.851	3.80	-79.747	110.126, 108.77[c]
		14.44								14.165	3.76	-105.38[e]	104.619[c], 97.309
	3.8												
							1.0000	0.0132	0.7612	57.851	3.80	-79.747	110.373, 108.77[c]
										14.165	3.76	-105.38[e]	104.619[c], 97.306
		174.2	C_2: 84.2	2.35854	64.913	4.913	0.9963	0.0859	4.9313	44.300	6.65	-34.931	102.54, 101.63[b]
		43.56					1.0036	0.0856	4.9132	44.262	6.65	-34.913	102.53, 101.643[b]
	6.6												
			C_3: 80.5	2.25490	63.673	3.673	0.9979	0.0642	3.6815	43.159	6.56	46.840[e]	103.163[c], 98.418
8							1.0020	0.0640	3.6739	43.163	6.56	46.836[e]	103.159[c], 98.420
		49	C_4: 69.8	1.95518	59.238	0.761	0.9999	0.0132	0.7612	49.746	3.52	-82.65	108.675[d]
		12.25										-62.149	106.074[d]
	3.5						1.0000	0.0132	0.7612	49.746	3.52	-82.65	108.675[d]
												-62.149	106.074[d]
		213.1	C_2: 84.0	2.35294	64.849	4.849	0.9964	0.0848	4.8667	213.59	7.30	-41.622	101.616[c], 99.417
		53.29					1.0035	0.8453	4.8493	213.58	7.30	-41.616	101.167[c], 99.416
	7.3												
			C_3: 80.0	2.24089	63.496	3.496	0.9981	0.0611	3.5031	213.35	7.30	-41.167	101.165[c], 99.417
9							1.0018	0.0609	3.4966	213.35	7.30	-41.165	101.167[c], 99.416
		81	C_4: 67.8	1.89915	58.227	1.772	0.9995	0.0309	1.7734	20.629	4.54	170.295	109.852[e], 110.295[c]
	4.5	20.25					1.0004	0.0309	1.7725	20.630	4.54	170.295	109.852[e], 110.295[e]
		60.84	C_2: 75.0	2.10084	61.575	1.575	0.9996	0.0275	1.5761	61.576	3.92	28.423	104.212
		15.21								61.257	3.91	-40.525	100.525[e]
							1.0003	0.0274	1.5755	61.575	3.92	28.424	104.211
10	3.9									61.257	3.91	-40.525	100.525[e]
			C_3: 68.8	1.92717	58.741	1.258	0.9997	0.0219	1.2584	61.258	3.91	28.741	104.370
										61.608	3.92	-40.419	100.419[e]

Comp	$^3J_{HH}$ [Hz]	Φ [deg]	δ_{Cn} [ppm]	δ_{Cn} [gaussx 10]	θ^{AIn} [deg]	θ^{AII} [deg]	1/h h [π]	r [π]	θ^{AIIn} [deg]	Φ [deg]	$^3J_{HH}$ [deg]	θ_{HnHn+1}+1 [deg]	φ_{Cn} [deg]
							1.0002	0.0219	1.2581	61.258	3.91	28.741	104.370
										61.608	3.92	-40.419	100.419[e]
		82.81	C_4: 74.9	2.09803	61.534	1.534	0.9996	0.0267	1.5346	331.38	9.10	146.931	106.53
		331.2								331.53	9.10	61.534	105.767
	9.1						1.0003	0.0267	1.5341	331.38	9.10	146.932	106.534
										331.53	9.10	61.534	105.767

a. ^{1}H, ^{13}C-NMR data ind. 8, 9; b. Six sets, c. tetrahedral angles characteristics for 5 rings on same set with dihedral angles, d. tetrahedral angle established for dihedral angle calculated from $\sin^{-1}\tan$ or $\tan^{-1}\sin$ function on same set, e. unit was build from set E instead C.

Step 2: The radius r of the cone inscribe on sphere at corresponding tangent point can be calculated from h or h^{-1} with eq. (6), then one angle of set AII with eq. (7) used for building units. Sometimes resulting directlly the vicinal angle or the dihedral angle, otherwise will be build units with seven sets angles.

$$r = [(a)^2\text{-}1]^{1/2}/(a) \quad (6)$$

Where a = h or 1/h.

$$\sin^{-1}r = \theta^{AIIn} \quad (7)$$

Where $\theta^{AIIn} \rightarrow$ units.

Units are build from calculated angle θ^{AIIn} in seven sets angles with possibility to increase to more units with set C, as a general rule used until now dihedral angles [6] are considered in close relationships with tetrahedral angles between set A, B and D, E or F, G if dihedral angle is in set B. Alternatively, six sets angles, three sets angles of unit U and three of unit S, in first case with angles higher as 5[deg] and in second case smaller as 5[deg], totally 14 sets angles. In this paper some units are build from sets D, E or F, G, or sets F, G are transformed in A, B, as well as no more as three units $C^{nNi} = U^{nNi}$, S^{nNi} are used [6].

Step 3: Characteristic equations for calculation dihedral angles – vicinal angles [6] and vicinal coupling constant [11] are used for choosing corresponding angles with calculated vicinal coupling constant values almost equals with recorded one.

Vicinal coupling constants are under two rules: *Case 1*: smaller vicinal coupling constant for *trans-ee* and *cis* stereochemistry and higher for *trans-aa* stereochemistry [6], iminocyclitols 1-6, 10, *Case 2*: higher vicinal coupling constant for *cis* stereochemistry and smaller for *trans-ee* and *trans-aa* vicinal coupling constant [11], iminocyclitols 7-9.

2.2. Calculated Dihedral θ_{HnHn+1}[deg] and Tetrahedral φ_{Cn}[deg] Angles on Seven and Six Sets Unit

In Table 1 are calculated dihedral θ_{HnHn+1}[deg] angles for imoncyclitols 1 - 10 from differences between two atoms of carbons $\Delta\delta_{CnCn+1}$[deg]. Dihedral angles are chosen from sets A and B having in mind relationship with tetrahedral angles φ_{Cn}[deg]. The presence of vicinal angles on sets A and B gives other possibility to calculate dihedral angles without building units (Table 1, comp 1, $^3J_{H2H3}$ 5.4[Hz]). In case of compound 2, vicinal angle ϕ[deg] under second rule [11] results from unit U^S calculated from unit U_1 with equation characteristic for transformation [12] U to S (ϕ = 9.64 or 9.79[deg]). Dihedral angles θ_{H3H4} and θ_{H2H3} of compounds 2 and 10 are calculated from sets D or G, using a different way for building units, relative to increased units from set C. In this case was reduced the number of units, method used also in Table 2 for calculation dihedral angles of 3 in close relationships with tetrahedral angles from carbon C_1 chemical shift δ_{C1}[ppm], or for compounds 9 and 7. In Table 1, compound 6, for a vicinal coupling constant of 4.6[Hz] unit was switch from set G to set A and angles are calculated from vicinal angles ϕ[deg]. Tetrahedral angle φ_{C4}[deg] for a vicinal coupling constant of 8.8[Hz] usually can be considered an angle from same sets with dihedral and vicinal angle, but must be contemplate as possible angle also increasing the unit from sets D, E or F, G.

2.3. Conic of Revolution and Dihedral Angle θ_{HnHn+1}[deg]

Cone of revolution, results from any Riemann surface of genus one embedded in the unit sphere S^3CR^4 as a flat torus, [1] can be used for calculation the distances $d_{HnHn+1i}[A^0]$ and bond length $l_{CnCn+1}[A^0]$. Distances between $H_nH_{n+1}{}^i$ can be calculated from rectangle geometry for *cis* stereochemistry and rhombus for *trans* stereochemistry [17] with conic approach or from equilateral triangles having as based $d_{HnHn+1}{}^i[A^0]$. In

the light of distances demonstration on the conic approach, the bond lengths $l_{CnCn+1}[A^0]$ for all stereochemistry are calculated with eq. 11. In case of rhombus geometry [17] *sin* instead of *cos* give the required diagonal for *trans-ee*^{3,2} and *trans-ee*^{4,1}.

Rectangle:

$$d_{HnHn+1}{}^{i} = 1.57x\cos^{1/2}\theta_{HnHn+1}[A^0] \quad (88)$$

Triangle:

$$d_{HnHn+1}{}^{i} = 0.5x[1.57x\cos^{1/2}(\theta_{HnHn+1}/2)][A^0] \quad (9)$$

$$d_{HnHn+1}{}^{i} = 1.57x\cos^{1/2}(\theta/2)[A^0] \quad (10)$$

where: $d_{HnHn+1}{}^{i}$ - distance between H_1 and $H_2{}^{i}$ in A^0,

$$l_{CnCn+1} = \{1.54x[1.57x\cos^{1/2}(\theta_{HnHn+1}/2)]\}^{1/2}[A^0] \quad (11)$$

where θ_{HnHn+1} – dihedral angles in deg.

3. Discussion

Dihedral angles θ_{HnHn+1}[deg] calculated from chemical shift δ [ppm] and vicinal coupling constant $^3J_{HH}$[Hz] with 3-sphere approach are usefully for determination phase angle of pseudorotation P[deg] and angle of deviation from planarity θ_m[deg]. [6, 13].

Dihedral angles θ_{HnHn+1}[deg] calculated with conic projection eq. (1)-(3) ensures the relationship between dihedral θ_{HnHn+1}[deg] and tetrahedral φ[deg] angles under *sin and tan functions in opposite*, [10] a model for calculation used to date for five and six membered [6] ring carbasugar. Higher number of units for choosing dihedral angle θ_{HnHn+1}[deg] with values almost equal with dihedral angle calculated only from recorded vicinal coupling constant have in opposite with tetrahedral φ_{Cn}[deg] angles a complicatedly system for establishing the trigonometric equations. The main question, are dihedral and tetrahedral angles in opposite under strict sin and tan trigonometric functions for building units or simply relationships between sets A, B and D, E, and F, G ensure sin *versus* tan functions? Probably the conic projection manifold is the answer.

Conic projection as manifold proves that in case of radius of the cone inscribes on sphere at tangent point (r), calculated from height of cone h or inverse of height h^{-1}, *the tan function of h is equal with sin function of* h^{-1} (Eq. (12)). [7].

$$60 - \cos^{-1}R_m = \theta^{AN1} = \sin^{-1}r,\ \theta^{AI1} = \theta^{AII1} \quad (12)$$

with N = I, II, n = 1 – 6.

A program for calculations dihedral θ_{HnHn+1}[deg] and tetrahedral φ_{Cn}[deg] angles in opposite [10] from sin and tan functions, can be simplified using first the trigonometric equations ensuring relationship between dihedral θ_{HnHn+1}[deg] and tetrahedral φ_{Cn}[deg] on seven sets angle and six angles, and second can be chose in opposite dihedral θ_{HnHn+1}[deg] with tetrahedral φ_{Cn}[deg] angles.

Euclidean coordinates in (n+1) space (Figure 4): *0-Sphere*: pair of points (c-r, c+r), boundary of a line segment (1-ball); *1-Sphere*: Abelian *Lie grup structure* U(1), circle group; *2-Sphere 3-dimensional Euclidean space (3-ball)*; 3-Sphere: also namely Glome, 4-dimension Euclidean space. Cylindrical coordinates having conic coordinates as limited case, surface of revolution with zero Gaussian curvature, giving the possibility to analyzed their geodesics on the equivalent flat surface are characteristic for torus. Unroll cone cut along a meridian become straight lines in the plane, and represent a way to translate in two-dimension. [14] Conic projection *versus* conic section, as published already are coordinates used for hypersphere tessellation [12, 15], a map projection that transform point from a sphere in tangent or secant of cone that is wrapped around the sphere [5].

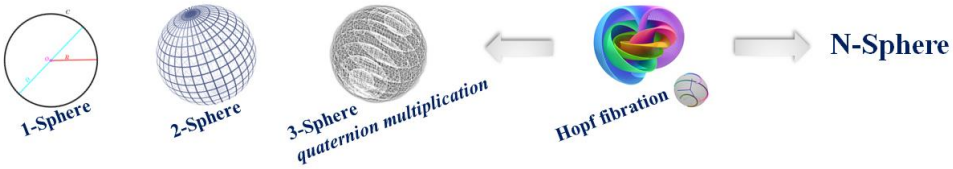

Figure 4. *Euclidian coordinates in (n+1) space.*

From the trigonometric point of view vicinal ϕ[deg] angle is in close relationship with dihedral θ_{HnHn+1}[deg] angle on two sets angles, two intersecting circles, real Hopf fibration, relative to R^4-complex Hopf fibration where both angles can be vicinal ϕ[deg] or dihedral θ_{HnHn+1}[deg] angles resulting two vicinal coupling constant $^3J_{HH}$[Hz]. A hole inside of sphere gives two tori, 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. The transformation from sphere to torus simulate better by building unit S from *trans-ee*^{3,2} of unit U, and represent a good explanation for R^{16} octonionic Hopf fibration, double of quaternionic R^7, for all *cis*, *trans-ee*, *trans-aa* stereochemistry, observed on two units representation with six sets angles or four sets angles from the strict trigonometric point of view. Since trigonometric equations don't differentiate between *trans-ee*^{4,1} and *trans-ee*^{3,2}, algebraic equations

have different values and place angles on two units U and S with first angles higher or smaller as 5[deg]. [16].

Polyhedron equation [13] under Fibonacci numbers F^n, golden ratio φ and golden triangle, can be used for transforming tetrahedral angles φ_{Cn}[deg] presented in Table 2 from calculated angles in close relationships with dihedral angle, in predicted angles in agreement with five membered ring trigonometry, *i.e.* compound 2, φ_{C2} 104.94[deg] under polyhedron equation become 101.243[deg] and φ_{C2} 105.729[deg] under polyhedron equation become 106.796[deg]. Based on other conformational analysis [13] on compound 2, in case of calculated phase angle of the pseudorotation E_3 and $E_2 - {}^3T_2$ in close relationship with dihedral angles on seven sets angles, E_3 conformation gives angles for $C_{1,4}$ around 105 and for $C_{2,3}$ around 104[deg] on seven sets angles. Calculated tetrahedral angles φ_{Cn}[deg] can be considered transition states (TS), or only values result from six sets angles must be considered, polyhedron transformation giving values comparable with six sets angles. Since between E_3 and $E_2 - {}^3T_2$ are not expected higher differences on values of tetrahedron angles, probably one from two methods must be applied as well as at list the values of tetrahedron angles to be in line with five membered ring geometry [13].

As observation on Table 2, dihedral angles 10-θ_{H3H4}[deg] with $^3J_{HH}$ 9.1[Hz] and *trans-aa* 146.9[deg] and *trans-ee* 61.53[deg] stereochemistry are calculated with positive sign from vicinal angle ϕ 331.3 or 331.5[deg], angles characteristic for L-stereochemistry, relative to 82.81[deg] with only one possible positive dihedral angle, but inexistent on first units. Second vicinal angle giving negative sign for D-stereochemistry.

Conic of revolution on calculation of the distances $d_{HnHn+1i}[A^0]$ and bond length $l_{CnCn+1}[A^0]$ gives the relationship between dihedral angle and *cis*, *trans*- stereochemistry on rectangle and equilateral triangle.

4. Conclusions

Dihedral angles θ_{HnHn+1}[deg] are calculated with conic projection as manifold from differences between two atoms of carbon $\Delta\delta_{CnCn+1}$[ppm] and vicinal coupling constant $^3J_{HH}$[Hz], or for carbon chemical shift δ_{Cn}[ppm] and vicinal coupling constant $^3J_{HH}$[Hz] in close relationships with tetrahedral angles φ_{Cn}[deg] on seven or six sets angles unit(s). In attempt to reduce the number of units calculated by hand, relative to units build through set C, in few cases units are constructed also from sets F and G. Probably a model for calculation all the possible dihedral angles with values almost equals with recorded that must be applied for calculation the number of units until the calculated angles are almost equals with angles on first unit. [16].

The relationships between dihedral θ_{HnHn+1}[deg] and tetrahedral φ_{Cn}[deg] angles in opposite from the trigonometric point of view was demonstrated with conic projection.

Conic of revolution on calculation of the distances $d_{HnHn+1i}[A^0]$ and bond length $l_{CnCn+1}[A^0]$ with eq. 8-11 was point out.

Abbreviations

RMN data Nuclear Magnetic Resonance Data

Conflicts of Interest

The authors have not conflicted of interest.

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