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Research Article

Stereochemistry of D, L-ribitol Iminocyclitols Between 4 and 2 Dimensions

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Abstract

The transformation from 4D to 3D and 2D exemplified recently with Lie algebra and Hopf fibration on *cis*, *trans-ee*, *trans-aa* stereochemistry, now is demonstrated with hypersphere trigonometric equations for calculation dihedral angles θ_{HnHn+1} [deg] from carbon chemical shift δ_{Cn} [ppm], then the vicinal angle ϕ [deg] and the other five possible dihedral angles θ_{HnHn+1} [deg] for one known vicinal coupling constant $^3J_{HnHn+1}$ [Hz]. *Cis*, *trans-ee* and *trans-aa* stereochemistry placed on six sets angles on two units have *trans-ee*^{4,1} stereochemistry under 2D dimension on unit S and *trans-ee*^{3,2} stereochemistry particularized with algebraic equations on unit U under 4D. Both *trans-ee* stereochemistry representing a great example for continuum transformation for hypersphere to torus. B^2 root system $\theta = 150$ [deg] as alternative model for building unit under Hopf fibration, along A^2 root system $\theta = 120$ [deg] unit will be disclosed, the second one ensuring also relationships between dihedral θ_{HnHn+1}[deg] and vicinal angles ϕ[deg]. Three pair of sets angles representative for five membered rings simulated for a vicinal coupling constant, sets A, B - dihedral and vicinal angles, set C used to build unit U_2 with set A and B calculated with $3\alpha + 2\beta$, and pair of sets A and B of unit S_1 calculated with $3\alpha + 3\beta$.

Keywords

Hypersphere Coordinates, Hopf Fibration, A2 Root System - Lie Algebra, B2 Root System - Hasic, Stereochemistry, Dihedral Angles

1. Introduction

Algebra of rotation in 3-space build into the Hopf map, set of unit length quaternions in R^4 viewed as points, is 3-Sphere S^3. The 4^{th} dimension known as space - time, embedding three-dimensions (3D) geometry into four-dimensions (4D) space where the fourth dimension is time (t). [1] Six dihedral angles θ_{HnHn+1} [deg] with *cis*, *trans* stereochemistry on three concentric cons under Hopf fibration can be visualized as two sets angles each with six *cis*, *trans-ee*, *trans-aa* stereochemistry having characteristics vicinal angles ϕ [deg] for every stereochemistry. The vicinal angle with *trans-ee*^{3,2} stereochemistry on unit U became first angle θ^{SA1} [deg] on unit S, totally six sets angles on two units point out the transformation from hypersphere to torus from 4D to 2D [2].

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2. Results

Dihedral angles θ_{HnHn+1} [deg] can be calculated from carbon chemical shift δ_{Cn} [deg] with hypersphere equations in 4D for *cis*, *trans-ee*[3, 2], *trans-aa* stereochemistry (Table 1) and 2D for *trans-ee*[4, 1] stereochemistry (Table 1, entry 3, 4) as sine or tangent functions generalized equations, and alternatively from 4D to 2D in function of the functional groups and stereochemistry.[3] Equations obtained in attempt to demonstrated the relationship between biological activity and trigonometrical equations [4] around the five membered ring iminocyclitols. Trifluoroacetate salt β-L-ribitol with decyl at C_1 have all trigonometric equation in 2D as tangent function, di alkyl - α, D- and β, L-ribitol have 4D trigonometric equations at C_1 and C_2, and 2D at C_2, C_3. Deprotection of the isopropylidene protective group change the trigonometric equations from 4D to 2D as cosine function at C_1, C_2, C_3 and tangent function at C_4. [5] In Table 1 are calculated dihedral angles corresponding to eq. 1 from carbon chemical shift, thus can be calculated the vicinal angle ϕ [deg] then the dihedral angles θ_{HnHn+1} [deg] from eqs. 2-4.

Trigonometric equations (Eq. 1-4), torus and invers of torus, for calculation dihedral angles θ_{HnHn+1} [deg] with *trans-ee* stereochemistry don't differentiate between *trans-ee*[3, 2] and *trans-ee*[4, 1] in comparation with algebraic equations (Eq. 7-16), able to give different values for *trans-ee*[4, 1] and *trans-ee*[3, 2] stereochemistry.

2.1. Trigonometric Equations

$$\theta HnHn+1 = f(\phi[deg])\ [deg]$$

$$\theta_{HnHn+1} = \sin^{-1}\cos\phi \quad (1)$$

$$\theta_{HnHn+1} = \tan^{-1}\sin(-\phi) \quad (2)$$

$$\theta_{HnHn+1} = \sin^{-1}\tan(-\phi) \quad (3)$$

$$\theta_{HnHn+1} = \sin^{-1}\cot(-\phi) \quad (4)$$

The vicinal angle ϕ [deg], angle calculated from vicinal coupling constant $^3J_{HH}$ [Hz] with eqs. 5 and 6 until now characteristics for *cis*, *trans-ee* stereochemistry for values smaller as 6 [Hz] and *trans-aa* stereochemistry for values higher as 6 [Hz], [6, 7] in case of isopropylidene protected L-ribitol with two alkyl chain at C_1 [5] the rule is switch, higher as 6 [Hz] for *trans-ee* stereochemistry and smaller as 6 [Hz] for *trans-aa* stereochemistry [5]. Four *cis*, *trans* possible combinations of vicinal angles simplified by the *cis* - *trans* relationship between dihedral angles θ_{HnHn+1} [deg].

2.2. Vicinal Angle

$$\phi = f(^3J_{HnHn+1}[Hz])$$

$$\phi = (2x^3J_{HH})^2 \quad (5)$$

$$\phi = (^3J_{HH})^2 \quad (6)$$

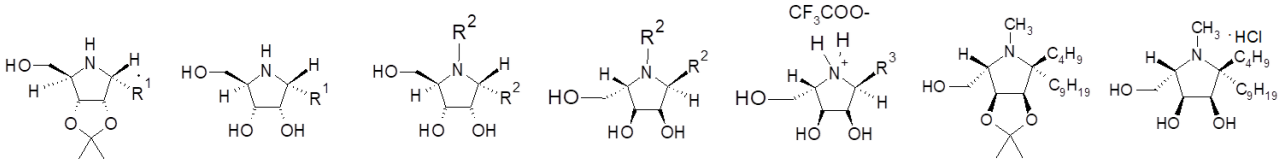

Figure 1. *Iminocyclitols with D- and L-ribitol stereochemistry bearing monoalkyl and di alkyl chain at C1.*

Table 1. *Dihedral angles θHnHn+1 [deg] calculated for iminocyclitols 1 - 7 from carbon chemical shift δCn [deg] with hypersphere equations.*

Entry	Comp	$^3J_{HH}$[a] [Hz]	δ_{Cn}[a] [ppm]	R_m [gauss]	θ_{HnHn+1} [deg]	Φ [deg]	$^3J_{HH}$ [Hz]	θ_{HnHn+1} [deg]	Equations
1.	*1*	H_1H_2: 4.1 H_2H_3: 5.4 H_3H_4: (d H_3)	C_1: 55.8	1.5630	22.995	$(^3J_{HH}x2)^2$: 67.005	4.092	22.99, -42.63, -25.11, -22.99	4D-*cis*[6, 1]: θ_{HnHn+1} = $\tan^{-1}\sin[(\cos^{-1}1/R_m)/2]$
			C_2: 83.5	2.3389	-28.143	$(^3J_{HH}x2)^2$: 118.143	5.43	-28.14, -41.40, 32.338, 28.14	4D-*cis*[6, 1]: θ_{HnHn+1} = -$\tan^{-1}\sin[(\cos^{-1}1/R_m)/2]$
			C_3: 84.3	2.3613	-28.230	$(^3J_{HH}x2)^2$: 118.230	5.43	-28.23, -41.38, 32.47, 28.23	4D-*cis*[6, 1]: θ_{HnHn+1} = -$\tan^{-1}\sin[(\cos^{-1}1/R_m)/2]$
			C_4: 65.9	1.8459	-87.620[b]	$(^3J_{HH}x2)^2$: 2.379	0.7779	32.37, -2.37, -2.38, -32.37	4D- *trans-ee*[3, 2]: θ_{HnHn+1} = -2x{$\tan^{-}$

Entry	Comp	$^3J_{HH}$[a] [Hz]	δ_{Cn}[a] [ppm]	R_m [gauss]	θ_{HnHn+1} [deg]	Φ [deg]	$^3J_{HH}$ [Hz]	θ_{HnHn+1} [deg]	Equations
								87.62, -117.63, -117.62, -87.62	$^1\cos[(\sin^{-1}1/R_m)/2]\}^c$
			C_1: 57.4	1.6078	51.814	$(^3J_{HH}x2)^2$: 38.185	3.089	51.814, -51.859, -31.724, -51.813	4D-*cis*^{5,2}: θ_{HnHn+1} = 2x{$\tan^{-1}\sin[(\tan^{-1}R_m)/2]$}
		H_1H_2: 3.1	C_2: 71.5	2.0028	29.953	$(^3J_{HH}x2)^2$: 60.046	3.87	29.861, -40.906, -35.189, -29.953	4D-*cis*^{6,1}: θ_{HnHn+1} = $\tan^{-1}\sin[(\cos^{-1}1/R_m)/2]$
2.	*2*	H_2H_3: 3.9	C_3: 71.7	2.0084	29.861	$(^3J_{HH}x2)^2$: 60.138	3.87	29.861, -40.932, -35.039, -29.861	4D-*cis*^{6,1}: θ_{HnHn+1} = $\tan^{-1}\sin[(\cos^{-1}1/R_m)/2]$
		H_3H_4: 8.8	C_4: 66.8	1.8711	12.878 -167.121[b]	$(^3J_{HH})^2$: 77.121	8.78	12.91; -44.27; -13.217; -12.91 167.12, 107.12; -135.73, -75.73; -166.78, -106.78; -167.12, -107.12	4D-*trans-aa*^{6,1}: θ_{HnHn+1} = -0.5x{$\tan^{-1}\sin[\cos^{-1}(1/R_m)]/2\}^c$
									3D-*cis*^{6,1}: θ_{HnHn+1} = $\sin^{-1}[-1/[(\cos^{-1}1/R_m)/2]$
									2D-*cis*^{6,1}: θ = 2x$\tan^{-1}[1/(R_m/2)]$
			C_1: 63.7	1.7843	-2.049[3D] -1.631 -1.735	$(^3J_{HH}x2)^2$: 92.049 $(^3J_{HH}x2)^2$: 91.631 $(^3J_{HH}x2)^2$: 91.735	4.79 4.82 4.78	2.049, -44.98, 2.050, -2.049 1.631, -44.988, 1.631, -1.631 1.734, -44.986, 1.736, -1.735	4D-*cis*^{6,1}: θ_{HnHn+1} = 0.25x$\sin^{-1}\cos\{2x\tan^{-1}[1/(R_m/2)]\}$
									2D-*cis*^{6,1}: θ = 2x$\sin^{-1}(1/R_m)^{1/2}$
									4D-*cis*^{6,1}: θ_{HnHn+1} = 0.25x$\sin^{-1}\cos[2x\sin^{-1}(1/R_m)^{1/2}]$
3.	*3*	H_1H_2: 4.8 H_2H_3: 5.2	C_2: 72.5	2.0308	-19.140	$(^3J_{HH}x2)^2$: 109.14	5.22	-19.14, -43.371, 20.307, 19.14	4D-*cis*^{6,1}: θ_{HnHn+1} = $\tan^{-1}[2x\sin\{-\cos^{-1}[1/(R_m/2)]\}]$
		H_3H_4: (t H_3)	C_3: 74.0	2.0728	-15.230	$(^3J_{HH}x2)^2$: 105.23	5.12	-15.23, -43.975, 15.798, 15.23	2D-*cis*^{6,1}: θ_{HnHn+1} = -$\cos^{-1}[1/(R_m/2)]$
								32.12, -2.122, -2.125, -32.12	
								87.87, -117.87, -117.87, -32.12	4D- *trans-ee*^{3,2}: θ_{HnHn+1} = -2x{$\tan^{-1}\cos[(\sin^{-1}1/R_m)/2]\}^c$
								31.73, -1.73, -11.73, -31.73	
			C_4: 69.3	1.9411	-87.876[b] -91.738[b] -91.712[b]	$(^3J_{HH}x2)^2$: 2.1232 $(^3J_{HH}x2)^2$: 1.7388 $(^3J_{HH}x2)^2$: 1.7388	0.7285 0.6593 0.6543	88.26, -118.26, -118.26, -88.26	2D-*trans-ee*^{4,1}: θ_{HnHn+1} = -$[2x\sin^{-1}(1/R_m)^{1/2}]^c$
								31.71, -1.711, -1,712, -31.71	2D-*trans-ee*^{4,1}: θ_{HnHn+1} = -2x$\tan^{-1}[1/(R_m/2)]^c$
								88.28, -118.28, -118.28, -88.28	
		H_1H_2: 4.8				$(^3J_{HH}x2)^2$: 91.9579	4.79	-1.957, -44.983, 1.959, 1.957	3D-*cis*^{6,1}: θ_{HnHn+1} = $\sin^{-1}[-1/[(\cos^{-1}1/R_m)/2]$
4.	*4*	H_2H_3: 5.2	C_1: 68.4	1.9159	-1.957[3D] -2.4606 -2.5158	$(^3J_{HH}x2)^2$: 92.4606	4.80	-2.46, -44.973. 2.462, 2.46	2D-*cis*^{6,1}: θ = 2x$\tan^{-1}[1/(R_m/2)]$
		H_3H_4: bs				$(^3J_{HH}x2)^2$: 92.5158	4.80	-2.51, -44.972, 2.518, 2.51	4D-*cis*^{6,1}: θ_{HnHn+1} = 0.25x$\sin^{-1}\cos\{2x\tan^{-1}$

Entry	Comp	$^3J_{HH}$[a] [Hz]	δ_{Cn}[a] [ppm]	R_m [gauss]	θ_{HnHn+1} [deg]	Φ [deg]	$^3J_{HH}$ [Hz]	θ_{HnHn+1} [deg]	Equations
									$^{-1}[1/(R_m/2)]\}$ 2D-*cis*[6, 1]: $\theta = 2x\sin^{-1}(1/R_m)^{1/2}$ 4D-*cis*[6, 1]: $\theta_{HnHn+1} = 0.25x\sin^{-1}\cos[2x\sin^{-1}(1/R_m)^{1/2}]$
			C_2: 71.1	1.9915	-20.873	$(^3J_{HH}x2)^2$: 110.873	5.26	20.87, -43.056, 22.413, -20.87	4D-*cis*[6, 1]: $\theta_{HnHn+1} = 2x\tan^{-1}[2x\sin[-(\cos^{-1}(R_m/2)]$
			C_3: 72.7	2.0364	-20.629	$(^3J_{HH}x2)^2$: 110.632	5.259	20.62, -43.102, 22.114, -20.62	4D-*cis*[6, 1]: $\theta_{HnHn+1} = \tan^{-1}[2x\sin\{-\cos^{-1}[1/(R_m/2)]\}]$
			C_4: 70.9	1.9859	-87.982 -90.406 -90.405	$(^3J_{HH}x2)^2$: 2.0173 $(^3J_{HH}x2)^2$: 0.4068 $(^3J_{HH}x2)^2$: 0.4053	0.7101 0.3189 0.3183	32.01, -2.016, -2.019, -32.01 87.98, -117.98, -117.98, -32.01 30.406, -0.405, -0.406, -30.406 89.59, -119.58, -119.59, -89.59 30.40, -0.404, -0.406, -30.405 89.59, -199.59, -119.59, -89.595	4D- *trans-ee*[3, 2]: $\theta_{HnHn+1} = -2x\{\tan^{-1}\cos[-(\sin^{-1}1/R_m)/2]\}^c$ 2D-*trans-ee*[4, 1]: $\theta_{HnHn+1} = -[2x\sin^{-1}(1/R_m)^{1/2}]^c$ 2D-*trans-ee*[4, 1]: $\theta_{HnHn+1} = -[2x\tan^{-1}[1/(R_m/2)]^c$
			C_1: 63.3	1.7731	59.711	$(^3J_{HH}x2)^2$: 30.288	2.75	59.71, -26.76, -35.737, -59.71	4D-*cis*[5, 2]: $\theta_{HnHn+1} = \cos^{-1}\{\sin[(\tan^{-1}R_m)/2]\}$
			C_2: 72.1	2.0196	37.315	$(^3J_{HH}x2)^2$: 52.684	3.62	37.31, -38.49, -49.661, -37.31	4D-*cis*[5, 2]: $\theta_{HnHn+1} = \cos^{-1}\{\sin[2x\tan^{-1}(1/R_m)]\}$
			C_3: 73.4	2.0560	38.125	$(^3J_{HH}x2)^2$: 51.874	3.601	38.12, -38.19, -51.705, -38.12	4D-*cis*[5, 2]: $\theta_{HnHn+1} = \cos^{-1}\{\sin[2x\tan^{-1}(1/R_m)]\}$
5.	*5*	H_1H_2: 2.8 H_2H_3: 3.6 H_3H_4: 8.8	C_4: 63.9	1.7899	11.785 168.215 12.580 167.419	$(^3J_{HH})^2$: 78.214 $(^3J_{HH})^2$: 77.419	8.84 8.79	11.78, 44.389, -12.043, -11.78 168.21; -135.61, -75.61; -167.95, -107.95; -168.21, -108.22 12.58, -44.303, -12.875, -12.58 167.42, 107.42; -135.69, -75.69; -167.12, -107.12; -167.42, -107.42	4D-*trans-aa*[6, 1]: $\theta_{HnHn+1} = \tan^{-1}\sin\{[\tan^{-1}[1/(R_m/2)]/4\}$ 4D-*trans-aa*[6, 1]: $\theta_{HnHn+1} = 0.5x\{\tan^{-1}\sin[\cos^{-1}(1/R_m)]/2\}$
6.	*6*	H_2H_3: 7.3 H_3H_4: 4.5	C_1: 66.7	1.8683	-	-	-	-	
			C_2: 84.0	2.3529	-56.512	$(^3J_{HH}x2)^2$: 213.487	7.30	-56.51, 28.887, -41.419, 56.51	4D-*cis*[5, 2]: $\theta_{HnHn+1} = -\sin^{-1}\{\cos[(\tan^{-1}R_m)/2]\}$

Entry	Comp	$^3J_{HH}$[a] [Hz]	δ_{Cn}[a] [ppm]	R_m [gauss]	θ_{HnHn+1} [deg]	Φ [deg]	$^3J_{HH}$ [Hz]	θ_{HnHn+1} [deg]	Equations
		$H_5H_{5'}$: 11.1 H_5H_4: 2.9			37.004	$(^3J_{HH})^2$: 52.995	7.27	37.0, -38.610, -48.909, -37.0	4D-*cis*[5, 2]: ϕ = 2xsin^{-1}{2xtan[sin^{-1}(1/R_m)]/2]}
			C_3: 80.0	2.2408	-57.024	$(^3J_{HH}x2)^2$: 212.975	7.29	-57.02, 28.557, -40.451, 57.02	4D-*cis*[5, 2]: θ_{HnHn+1} = -sin^{-1}{cos[(tan^{-1}R_m)/2]}
					-	-	-	-	-
					69.66	$(^3J_{HH}x2)^2$: 20.34	4.51	-19.166, -21.759 69.66, -160.83, -158.24, -69.66	ϕ = tan^{-1}sin[tan^{-1}(Rm/2)/2]
			C_4: 67.8	1.8991	69.101	$(^3J_{HH}x2)^2$: 20.899	4.57	-19.632, -22.447 69.10, -160.36, -157.55, -69.10	4D-*trans-ee*[3, 2]: θ_{HnHn+1} = 2x{tan^{-1}sin[tan^{-1}(R_m/2)]
					6.841 173.159	$(^3J_{HH}x2)^2$: 83.159	4.55	6.84, -44.795, -6.890, -6.84 173.15, 113.16; -135.20, -75.20; -173.109, -113.11; -173.15, -113.16	4D-*trans-aa*[6, 1]: θ_{HnHn+1} = tan^{-1}{sin[tan^{-1}(1/R_m)]/2}/2
7.	*7*	H_2H_3: 3.9	C_1: 77.9	2.1820	-	-	-	-	-
			C_2: 75.0	2.1008	27.106	$(^3J_{HH}x2)^2$: 62.893	3.96	-41.674, -30.787	4D-*cis*[6, 1]: θ_{HnHn+1} = tan^{-1}sin[(cos^{-1}1/R_m)/2]
		H_3H_4: 9.1	C_3: 68.8	1.9271	6.759 173.24	$(^3J_{HH})^2$: 83.24	9.12	-44.80, -6.806 -135.2, -173.194	4D-*trans-aa*[6, 1]: θ_{HnHn+1} = tan^{-1}{sin[tan^{-1}(1/R_m)]/2}/2
		$H_5H_{5'}$: 12.5 H_5H_4: 3.0	C_4: 74.9	2.0980	6.293 173.70	$(^3J_{HH})^2$: 83.70	9.14	6.29, -44.826, -6.331, -6.29 173.78, -135.17, -173.66, -173.78	4D-*trans-aa*[6, 1]: θ_{HnHn+1} = tan^{-1}{sin[tan^{-1}(1/R_m)]/2}/2

δC [ppm], 1H 400 [MHz], 13C 75 [MHz]: 1-CDCl3, 2-D2O, 3-CDCl3, 4-CDCl3, 5-CD3OD, 6-CDCl3, 7-CD3OD; b. D-series - dihedral angle θH4H3[deg] must be negative; angles with trans stereochemistry calculated from δC4[ppm] are first angles from three possible calculated from dihedral angles characteristics equations 1 - 4; c. negative sign characteristic for D stereochemistry; vicinal angle higher as 90[deg] gives negative sign.

Dihedral angles for iminocyclitols *1* - *7* (Figure 1) calculated from carbon chemical shift δ_{Cn}[deg] with hypersphere equations *1* - *6* are presented in Table 1. Iminocyclitols *1* - *7* are characterized with NMR analysis: 1H, 13C, COSY, HMQC, IR and MS. [5, 7] In Supporting information are given the NMR spectra of iminocyclitols *6* and *7* and IR spectra of *7*.

Four cases result from combinations of eq. 5, 6 for calculation vicinal angle ϕ[deg] from vicinal coupling constant $^3J_{HH}$ [Hz] and eq. 1-4 for calculation dihedral angles θ_{HnHn+1}[deg] from vicinal angle ϕ[deg] (Table 2). In other word, two main cases A and B from the *trans* stereochemistry point of view, eq. 5, 6 for *trans-aa* and *trans-ee* stereochemistry with corresponding *cis* stereochemistry. Under 3-Sphere trigonometric equations, Hopf Fibration theory: 180 rule for *cis*, *trans-aa* stereochemistry, and 120 - rule for *trans-ee* stereochemistry [8].

Table 2. *Four cis, trans cases result from vicinal coupling constant $^3J_{HH}$[Hz].*

***cis*: $^3J_{HH}$ < 6[Hz], *trans*: $^3J_{HH}$ > 6[Hz]**		***cis*: $^3J_{HH}$ > 6[Hz], *trans*: $^3J_{HH}$ < 6[Hz]**	
I. *cis, trans-ee*: $\phi = (2x^3J_{HH})^2$, *trans-aa*: $\phi = (^3J_{HH})^2$		II. *trans-aa*: $\phi = (2x^3J_{HH})^2$, *cis, trans-ee*: $\phi = (^3J_{HH})^2$	
IV. *trans-ee*: $\phi = (2x^3J_{HH})^2$, *cis, trans-aa*: $\phi = (^3J_{HH})^2$		III. *cis*, *trans-aa*: $\phi = (2x^3J_{HH})^2$, *trans-ee*: $\phi = (^3J_{HH})^2$	
A.		*B.*	
trans-ee: $\phi = (2x^3J_{HH})^2$	*trans-aa*: $\phi = (^3J_{HH})^2$	*trans-aa*: $\phi = (2x^3J_{HH})^2$	*trans-ee*: $\phi = (^3J_{HH})^2$
cis: $\phi = (2x^3J_{HH})^2$, $\phi = (^3J_{HH})^2$	cis: $\phi = (2x^3J_{HH})^2$, $\phi = (^3J_{HH})^2$	cis: $\phi = (2x^3J_{HH})^2$, $\phi = (^3J_{HH})^2$	cis: $\phi = (2x^3J_{HH})^2$, $\phi = (^3J_{HH})^2$

Java Script program for calculation dihedral angles from vicinal coupling constant reported in literature used only for *cis*, *trans-ee* stereochemistry eq. 5 and *trans-aa* stereochemistry eq. 6. [6] In the feature dihedral angles will be calculated from vicinal coupling constant with 3-Sphere approach using both equations for *cis*, *trans-ee* and *cis*, *trans-aa* stereochemistry, and in case of *trans-ee* stereochemistry the calculated angle will be transformed in dihedral angles under +/-90 [deg] for eq. 1 and +/-120 [deg] for eq. 2 - 4. In this light angle calculated to date for *trans-ee* stereochemistry are for example -118.44 [deg], -118.90 [deg] instead of -88.44 [deg], -88.99 [deg] (Table 3, entry 4 and 12, reference 9 and Table 1 reference 10, Table 1 reference 11, comp. 1, 3, 4, 7) [9-11]. The phase angle of the pseudorotation P[deg] can be established more easy with VISION molecular models in case of 1-α-methyl-1, 4-imino-1, 4-dideoxy-D-ribitol *2*, envelope E_3 -162 [deg] with the following dihedral angles 51.54, -33.46, -106.152 [deg], *trans-ee* H_3H_4 instead of *trans-aa* H_3H_4 stereochemistry, and with endocyclic torsional angles 8.46, -26.54, 13.848 [deg] and P -176.22 [deg], in first case the angle of deviation from planarity -35.18 and -26.597 [deg].[12] At this moment along the mentioned corrections the sign for D-ribitol *trans-aa* θ_{H3H4} stereochemistry is negative also for *trans-ee* θ_{H3H4} stereochemistry (Table 1, entry 3, reference 11) [13].

That must be mentioned again, Hopf fibration trigonometric equations ensure relationships between *cis* and *trans-aa* under 180[deg] and *cis* and *trans-ee* stereochemistry under 120[deg], exocyclic angles, relative to relationships between endocyclic angles under 120[deg] but with sign in opposite for *trans-ee* stereochemistry.[2] Molecular models indicates for a vicinal coupling constant 8.8[Hz] with *trans* stereochemistry and E_3 conformation[12] an angle of 107.1[deg] (Table 1, comp. 2), the rule used to date[8, 2] must be reconsidered. From calculated angles with *cis* stereochemistry results also angles with *trans-aa*$^{6,\,1\text{ or }5,\,2}$ stereochemistry under 180[deg], and also *trans-ee*$^{4,\,1\text{ or }3,\,2}$ stereochemistry under 120[deg]. In first case trigonometric relationships between angles: dihedral *cis* θ_{HnHn+1} - dihedral *trans* θ_{HnHn+1} - vicinal ϕ established the 180[deg] rule, in contradiction with 120[deg] rule used on stereochemistry.

Algebraic equations (7-16) under Lie algebra theory for *cis*, *trans* stereochemistry for case A (7 - 11) and case B (12 - 16) are agreement with Hopf trigonometric equations, [2] excepting *trans-ee* stereochemistry. Only algebraic equations differentiate between *trans-ee*$^{3,\,2}$ and *trans-ee*$^{4,\,1}$ stereochemistry, trigonometric equations giving same values with different sign. Algebraic equation with *trans-ee*$^{3,\,2}$ stereochemistry on unit U build unit S, thus an angle with *trans-ee*$^{3,\,2}$ stereochemistry on unit U in unit S is first angle of set A or $\phi_1/2$ of set B with uncertainly stereochemistry from the trigonometric point of view.

2.3. Algebraic Equations

$^3J_{HnHn+1} = f(\phi_1/2, \phi_2[deg])[Hz]$

case A:

$$\text{Cis/}trans\text{-}aa^{6,\,1}\text{: } {}^3J_{HH}{}^{6,\,1} = (60 + \phi_1{}^A/2)^{1/2}/m \quad (7)$$

$$\text{Cis/}trans\text{-}aa^{5,\,2}\text{: } {}^3J_{HH}{}^{5,\,2} = (\phi_2{}^A + \phi_1{}^A/2)^{1/2}/m \quad (8)$$

$$Cis/trans\text{-}ee^{3,\,2}\text{: } {}^3J_{HH}{}^{3,\,2} = (\phi_2{}^A - \phi_1{}^A/2)^{1/2}/m \quad (9)$$

$$\text{Cis/}trans\text{-}ee^{4,\,1}\text{: } {}^3J_{HH}{}^{4,\,1} = (\phi_1{}^A)^{1/2}/m \quad (10)$$

$$m = 1\ trans\text{-aa},\ m = 2\ cis\text{-},\ trans\text{-ee} \quad (11)$$

case B:

$$\text{Cis/}trans\text{-}aa^{6,\,1}\text{: } {}^3J_{HH}{}^{6,\,1} = [180 + (60 + \phi_1{}^A/2)]^{1/2}/m \quad (12)$$

$$\text{Cis/}trans\text{-}aa^{5,\,2}\text{: } {}^3J_{HH}{}^{5,\,2} = [180 + (\phi_2{}^A + \phi_1{}^A/2)]^{1/2}/m \quad (13)$$

$$Cis/trans\text{-}ee^{3,\,2}\text{: } {}^3J_{HH}{}^{3,\,2} = (\phi_2{}^A - \phi_1{}^A/2)^{1/2}/m \quad (14)$$

$$\text{Cis/}trans\text{-}ee^{4,\,1}\text{: } {}^3J_{HH}{}^{4,\,1} = (\phi_1{}^A)^{1/2}/m \quad (15)$$

$$m = 2\ trans\text{-aa},\ m = 1\ cis\text{-},\ trans\text{-ee} \quad (16)$$

The vicinal coupling constant $^3J_{H2H3}$ 7.3 [Hz] of iminocyclitol 6 with two alkyl chain at C_1 and isopropylidene protected have values for vicinal angle ϕ[deg] and dihedral angle θ_{HnHn+1}[deg] very close. From eq. 17 results angle θ[deg]

56.512 then the vicinal angle ϕ[deg] 213.467, or directly dihedral angle θ_{HnHn+1}[deg] -56.512 from which can be calculated the vicinal angle ϕ[deg].

$$4D\text{-}cis^{5,2}: \theta = (+/-)\ \sin^{-1}\cos[(\tan^{-1}R_m)/2 \quad (17)$$

As observation in Table 1, entry 5, with hypersphere equations in 4D are calculated dihedral angles for 2.8 and 3.6 [Hz], switching equation used for 2.8 [Hz] with equation used for 3.6[Hz] can be calculated in both cases the vicinal angle ϕ [deg].

$$\theta_{HnHn+1} = \tan^{-1}\cot(-\phi) \quad (18)$$

$$\phi = \sin^{-1}\cos(-\phi) \quad (19)$$

where θ_{HnHn+1} - dihedral angles [deg], ϕ - vicinal angle [deg].

Dihedral angles with sign in opposite results from Hopf fibration eqs. 1 and 18. Equation 18 ensuring a real relationship dihedral θ_{HnHn+1}[deg] - vicinal ϕ[deg] angles, since corresponding equation 19 to 1 gives only vicinal angle ϕ [deg].

Until considering equation 18 *cis* dihedral angles θ_{HnHn+1} [deg] are transformed in *trans-ee* stereochemistry under 120 [deg] rule, huge number of calculate *trans-ee* dihedral angles θ_{HnHn+1} [deg] with positive and negative sign, sometimes from unexpected vicinal coupling constant created a debate on the method for choosing *trans-ee* dihedral angles θ_{HnHn+1}[deg]. Having in mind *trans-aa* stereochemistry under 180[deg] relative to *cis* dihedral angles θ_{HnHn+1}[deg], probably both method for calculation can be considered for *trans-ee* stereochemistry.

3. Discussions

Six dihedral angles θ_{HnHn+1}[deg] with *cis*, *trans* stereochemistry can be represented on three concentric cons and calculated the vicinal angles ϕ[deg] for every stereochemistry with algebraic equations (7-16), or dihedral angle θ_{HnHn+1} [deg] with trigonometric equations (1-4) from vicinal angle ϕ[deg], angle calculated from vicinal coupling constant $^3J_{HH}$ [Hz]. From carbon δ_{Cn} [ppm] and / or proton δ_{Hn}[ppm] chemical shift with manifold equations [14] can be calculated one angle for building unit U and S, six sets angles on two units. First angles of set A and B are higher as 5[deg] in unit U and smaller as 5 [deg] in unit S. The transformation between unit U to unit S through vicinal angle ϕ[deg] characteristic for *trans-ee*^{3,2} stereochemistry calculated from unit U, gives fist angle of unit S, as results from algebraic equations 9, 14. From the mathematic point of view a hole outside of sphere gives two tori, analog to building unit S from *trans-ee*^{3,2} stereochemistry of unit U, continuum transformation from hypersphere to torus, *demonstrated now with hypersphere equations* along to Hopf fibration and Lie algebra. As main observation, under trigonometric equations *cis*, *trans-aa* stereochemistry is under 180 [deg] rule and *trans-ee* stereochemistry under 120[deg], borderline between spherical geometry and probably equilateral triangle geometry, between cyclide and spherical geometries. Only *trans-ee*^{4,1} stereochemistry is under 2D dimension on unit S, *trans-ee*^{3,2} stereochemistry resulting from unit U is under 4D, analog with *cis* and *trans-aa* stereochemistry (Figure 2).

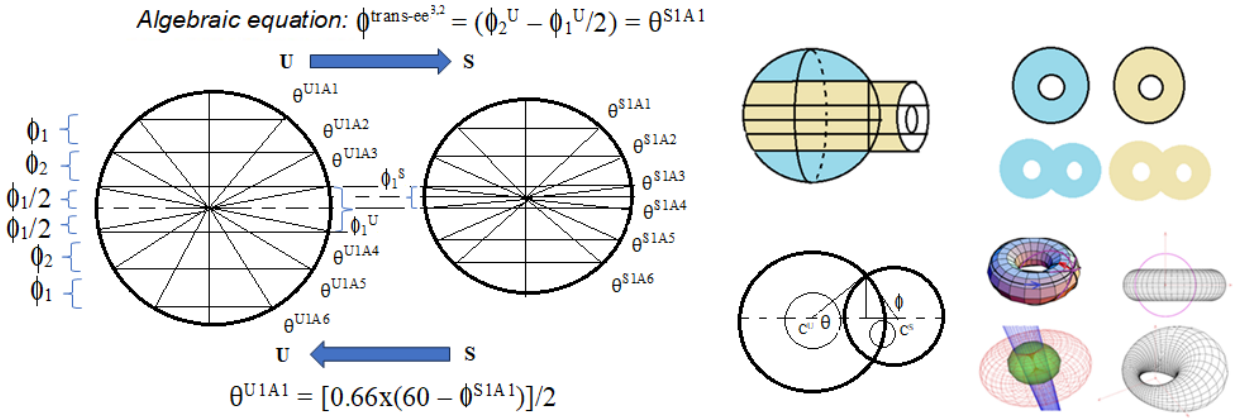

Figure 2. *Trans-ee*^{3,2} *and trans-ee*^{4,1} *stereochemistry and transformation from 4D to 2D.*

In accord with Hopf fibration, *trans-ee* stereochemistry is placed on two pairs of three circles, totally six sets angles. First pair of three sets angles having first angles of set A and B higher as 5[deg] namely unit U with three sets angles, and first angles of second pair of three sets angles smaller as 5[deg] namely unit S with three sets angles, values established based on experimental data used to date, at borderline is possible to increase the interval of values as calculated theoretical. At list the transformation from unit U to S and unit S to U with characteristics equations already published [2] gives the intervals of angles characteristic for unit U or S, and not the values of the *trans-ee* vicinal angle ϕ[deg]. In fact, the rules of calculation vicinal coupling constant for cis, trans-ee and trans-aa change the interval, and the transformation from S to U shown a distribution of first angles between S and U units as presented in Table 3.

Table 3. *Interval of values for transformation U to S and S to U.*

Entry	Units	θ^{A1}	θ^{B1}	θ^{A1}	θ^{B1}	θ^{A1}	θ^{B1}	θ^{A1}	θ^{B1}	θ^{A1}	θ^{B1}	θ^{A1}	θ^{B1}
1.	S	0.1	29.9	1	29	6	24	9	21	14	16	15	15
2.	U	19.96	10.03	19.66	10.33	18	12	17	13	15	14	15	15

B^2 root system θ = 150 [deg], can be an alternative to A^2 root system θ = 120 [deg], [15] but can be also transform into a method for calculation set C from sets A or B, and now at list for building unit S from unit U (Figures 3, 4).

Three pair of sets angles representative for five membered rings are simulated in Figure for a vicinal coupling constant of 4.1 [Hz] with *cis*-H_1H_2 stereochemistry, A, B - dihedral and vicinal angles, set C used to build unit U_2 with set A and B bearing tetrahedral and internal angles calculated with 3α + 2β, and pair of sets A and B of unit S_1 calculated with 3α + 3β (Figure 4).

$$-\alpha - \beta: [-(-90) - 69.112^{UA}] = 20.887^{UB}[deg]$$

$$-2\alpha - 2\beta: [-(-2x90) - 2x69.112^{UA}] = 41.776^{UC}[deg]$$

$$-3\alpha - 3\beta: [-(-3x90) - 3x69.112^{UA}] = 62.66^{SA}[deg]$$

3-Different methods for visualizing the "close universe" S^3: 1. Slicing method, 2. Suspension method, 3. Gluing cones together. The first one, non-Euclidean geometry of the closed Friedmann solution to Einstein's field geometry presented as a sphere embedded in 4-Euclidean space - a topological presentation. S^2 resulting from S^3 at intersection with a hyperplane $W = W^0$, once W increased from -R to R result the points of S^3 as the points of a family of S^2 growing from zero to R. 2-Sphere can be sliced up by planes into circles, and the circle can be sliced by lines into 0-spheres [16].

$$S^3: X^2 + Y^2 + Z^2 = R^2$$

$$S^2: X^2 + Y^2 + Z^2 = R^2 - W_0^2$$

$$W_0^2 < R^2, \text{ a single point } X = Y = Z = 0$$

Trigonometric equations for calculation dihedral angles from vicinal angles, R^{16} - octonionic Hopf fibration[12] for all stereochemistry, two angles with *trans-ee* stereochemistry from unit S and six stereochemistry from unit U, a great simulation of continuum transformation from 4D to 2D. Real Hopf fibration for calculation dihedral angle θ_{HnHn+1}[deg] from vicinal angle ϕ[deg], angle calculated from only one vicinal coupling constant $^3J_{HH}$[Hz] or R^4 complex Hopf fibration for calculation angles of set A and B for two possible vicinal coupling constants: $\theta^{NA} = \theta_{HnHn+1}$, $\theta^{NB} = \phi$, resulting $^3J_{HH}{}^B$[Hz] or $\theta^{NB} = \theta_{HnHn+1}$, $\theta^{NA} = \phi$, resulting $^3J_{HH}{}^A$[Hz].

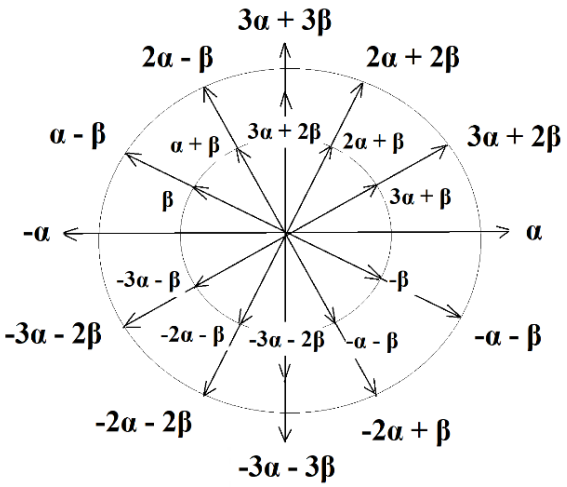

Figure 3. *B2 root system for calculation dihedral angles on first circle and angles of set C and transformation from unit U into unit S on second circle.*

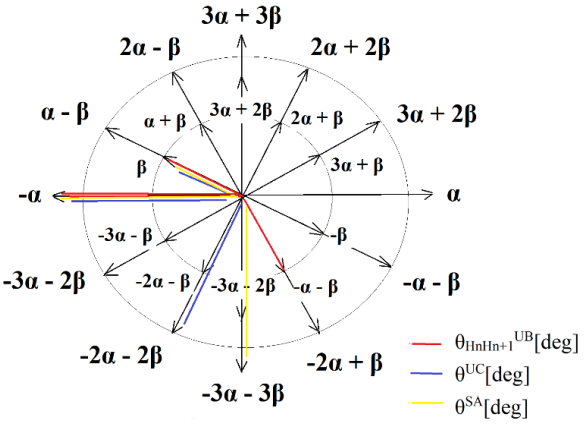

Figure 4. *B2 root system exemplified for a vicinal coupling constant of 4.16[Hz] and vicinal angle of ϕ 69.112 [deg].*

Basical equation - is a real Hopf fibration [17] - considering angle of set A vicinal angle and angle of set B dihedral angle. R^{16} - octonionic Hopf fibration for all stereochemistry. Other

two dihedral angles can be calculated from invers of torus equations, tangential space. Totally six dihedral angles from two characteristics equations for calculation vicinal angles from only one vicinal coupling constant. Higher number of dihedral angles calculated from only one vicinal coupling constant are reduced by the stereochemistry of iminocyclitol: negative H_4H_3 for D ribitol and positive H_3H_4 for L ribitol; by the relationship with corresponding tetrahedral angle, [18] and by the phase angle of the pseudorotation established with VISION molecular models. Two iminocyclitols, deprotected D-ribitol (*2*) bearing only one substituent at C_1, and isopropylidene protected L-ribitol (*6*) with two alkyl chain at C_1 have vicinal coupling constant in opposite: smaller values for *trans-aa* stereochemistry for iminocyclitol *6* and higher values for *cis* stereochemistry, unusually but now unknown, with dihedral angle under case II or III [19].

4. Conclusions

Hypersphere trigonometric equations demonstrated once again the transformation from 4D to 2D, [20] the transformation from hypersphere to torus, in case of cis - *trans* stereochemistry with continuum transformation from sphere to torus. Three concentric cons ensuring all *cis* - *trans* stereochemistry, a hole outside of hypersphere, in fact two cones outside of hypersphere giving tori, a topological modification simulate by stereochemistry.

Dihedral angles θ_{HnHn+1}[deg] can by calculated from vicinal coupling constant $^3J_{HH}$ [Hz] with eq. 5, 6 and circles of sphere and cyclide eq. 1-4, totally six dihedral angles θ_{HnHn+1}[deg] with required sign and stereochemistry from only one vicinal coupling constant $^3J_{HH}$[Hz], reduced by stereochemistry of iminocyclitol, relationship with tetrahedral angles, and conformation and configuration [3, 18, 19].

Abbreviations

RMN	Muclear Magnetic Resonance

Author Contributions

Carmen-Irena Mitan: Conceptualization, Methodology, Resources

Emerich Bartha: Conceptualization, Methodology, Resources

Conflicts of Interest

The authors declare no conflicts of interest.

References

[1] P. C. Caplan, Tessellation and interactive visualization of four-dimensional space time geometries, *Computer - Aided Design* 2025, 178, 103792.

[2] C.-I. Mitan, E. Bartha, P. Filip, R. Moriarty, Nuclear Magnetic Resonance Spectroscopy - Recent Research and Applications, chapter book: Dihedral and tetrahedral angles of small rings calculated from Vicinal coupling constant and chemical shift with 3-Sphere approach, IntachOpen ISBN 978-1-83635-220-4. http://dx.doi.org/10.5772/intechopen.1009208

[3] C.-I. Mitan, P. Filip, E. Bartha, C. Draghici, M.-T. Caproiu, R. M. Moriarty, Stereochemistry of *cis* - *trans* vicinal coupling constant $^3J_{HH}$[Hz] on 3-Sphere approach with application in conformational analysis, ACS Spring, San Diego march 23 - 27, Sci-Mix CARB - ANYL 632, ID 4175485; https://doi.org/10.1021/scimeetings.5c11052

[4] C.-I. Mitan, E. Bartha, P. Filip, Hypersphere coordinates on calculation of the dihedral angles from carbon chemical shift, *Bulletin of Romanian Chemical Engineering Society* 2022, 9(2), 151; ISSN 2360-4697.

[5] R. M. Moriarty, C.-I. Mitan, B. Gu, T. Block, Hypersphere and Antiviral Activity of three Alkyl Chain Imnocyclitols with D and L Ribitol Stereochemistry, *American Journal of Heterocyclic Chemistry* 2023, 9(1), 9-24. *SciencePG*: https://doi.org/10.116481/jajhc20230901.12

[6] C.-I. Mitan, E. Bartha, P. Petru, C. Draghici, M.-T. Caproiu, R. M. Moriarty, Manifold inversion on prediction dihedral angle from vicinal coupling constant with 3-sphere approach, *Rev. Roum. Chim.* 2023, 68, (3-4), 185; https://doi.org/1-.33224/rrch.2023.68.3-4.08

[7] R. M. Moriarty, C. I. Mitan, N. Branza-Nichita, K. P. Phares, D. Parrish, exo-Imino to *endo*-Iminocyclitol Rearrangement. A general route to five membered antiviral azasugars. *Organic Lett.* 2006, 8, 3465; https://doi.org/10.1021/ol1061071r

[8] E. Bartha, C.-I. Mitan, P. Filip 3-Sphere Torsional Angles and Six Membered Ring Conformation, *American Journal of Quantum Chemistry and Molecular Spectroscopy* 2023, *7*(1), 9.

[9] C.-I. Mitan, E. Bartha, P. Petru, Relationship between tetrahedral and dihedral on hypersphere coordinates, *Rev. Roum. Chim.* 2023, 68(5-6), 261; https://doi.org/1-.33224/rrch.2023.68.5-4.09

[10] C.-I. Mitan, E. Bartha, C. Draghici, M.-T. Caproiu, P. Filip, R. M. Moriarty, Tetrahedral angles of five membered ring iminocyclitols with ribitol stereochemistry beyond the dihedral angles, *Rev. Roum. Chim.* 2022, 67(3), 165; https://doi.org/1-.33224/rrch.2022.68.3.04

[11] C.-I. Mitan, E. Bartha, P. Filip, M.-T. Caproiu, C. Draghici, C. Deleanu, V. Dragutan, R. M. Moriarty, Conic projection as manifold and 3-sphere dihedral angles θ_{HnHn+1}[deg] under homotopy, *Sci. J. Chem.* 2026, 14(1), 12; https://doi.org/10.11648/j.sjc.20261401.12

[12] C.-I. Mitan, E. Bartha, P. Filip, V. Dragutan, I. Dragutan, C. Deleanu, C. Draghici, M.-T. Caproiu, R. M. Moriarty, 3-Spherical conformation insight into iminocyclitols with 1-α-D-ribose and 1-β-L-ribose stereochemistry under homotopic behavior of nuclear magnetic resonance data, *Sci. J. Chem* 2026, 14(1), 1-11. *SciencePG*: https://doi.org/10.11648/j.sjc.20261401.11

[13] E. Bartha, C.-I. Mitan, C. Draghici, M.-T. Caproiu, P. Filip, L. Tarko, R. M. Moriarty, Program for prediction dihedral angle from vcinal coupling constant with 3-sphere approach, *Rev. Roum. Chim.* 2021, 66(2), 179; https://doi.org/1-.33224/rrch.2021.66.2.08

[14] C.-I. Mitan, E. Bartha, P. Filip, C. Draghici, M.-T. Caproiu, R. M. Moriarty, Java Script programs for calculation of dihedral angles with manifold equations, *Science Journal of Chemistry* 2024, 12(3), 42; https://doi.org/10.11648/j.sjc.20141203.11

[15] A. Hasic, An introduction to Lie group, Advances in linear algebra & matrix theory 2021, 11, 67; www.scirp.org/journal/alamt

[16] M. A. Peterson, Dante and the 3-Sphere, *Am. J. Phys.* 1979, *47*, 1031; https://doi.org/10.1119/1.11968

[17] C.-I. Mitan, E. Bartha, C. Draghici, M. T. Caproiu, P. Filip, R. M. Moriarty, Hopf fibration on relationship between dihedral angle θ_{HnHn+1}[deg] and vicinal angle ϕ[deg], angles calculated from NMR data with 3-sphere approach and Java Script, *Science Journal of Chemistry* 2022, 10, 21. *SciencePG*: https://doi.org/10.11648/j.sjc.20221001.13

[18] C.-I. Mitan, E. Bartha, P. Filip, C. Draghici, M.-T. Caproiu, R. M. Moriarty, 3-Sphere tetrahedral angles and *cis* - *trans* stereochemistry of vicinal coupling constant $^3J_{HH}$[Hz], ACS Spring, San Diego march 23 - 27, CARB 617, ID 4189960; https://doi.org/10.1021/scimeetings.5c11050

[19] C.-I. Mitan, E. Bartha, P. Filip, C. Draghici, M.-T. Caproiu, R. M. Moriarty, 3-Sphere dihedral angles under wave character of the NMR data with applications on conformational analysis, ACS Spring, San Diego march 23 - 27, CARB 623, ID 4175487; https://doi.org/10.1021/scimeetings.5c11051

[20] M. S. ElBialy, J. Math. Anal. Appl. 2007, 332, 631; https://doi.org/10.1016/j.jmaa.2006.09.079