

## Research Article

# Java Script Programs for Calculation of Dihedral Angles with Manifold Equations

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## Abstract

Java Script programs for calculation dihedral angles from NMR data with manifold equations of 3-Sphere approach: rectangle, Villarceau circles of cyclide (Torus – Dupin Cyclide), polar equations, Euler-Conic. Manifolds are curves or surface in higher dimension used for calculation of dihedral angles under wave character of NMR data, carbon and/or proton chemical shift  $\delta_{Xn}$ [ppm] and vicinal coupling constant  $^3J_{HnHn+1}$ [Hz]. 3-Sphere approach for calculation of the dihedral angles from NMR data in four steps: 1. Prediction, or more exactly calculation of the dihedral angles from vicinal coupling constant with trigonometric equations, 2. Calculation of the dihedral angles from manifold equations; 3. Building units from angle calculated with one of the manifold equations; 4. Calculation the vicinal coupling constant of the manifold dihedral angle. In this paper are presented Java Script programs of step 2 and from step 3 only the Java Script program for calculation of seven sets angles. The bond distances  $l_{CnCn+1}[A^0]$  between two atoms of carbon are under different polar equations (*i.e.* limaçons or cardioid, rose or lemniscate), our expectation was to find different manifold equations for calculation the best angle, differences are smaller but can be find sometimes a preferred one for a vicinal coupling constant. 3-Sphere approach has the advantages of calculation from vicinal angle or/and chemical shift the dihedral angle, tetrahedral angle and the bond distance  $l_{CnCn+1}[A^0]$ , with application on conformational and configurational analysis.

## Keywords

Manifold, Rectangle, Villarceau Circles, Euler-Conic, Hopf Fibration, Lie Algebra, 3-Sphere, Dihedral Angles, Java Script

## 1. Introduction

Curve or surface generalized in higher dimensions are named manifold, are applied in classical mechanics, general relativity and quantum field theory using elements of algebra, topology, and analysis. [1] A manifold can be locally Euclidean space, but also smooth (Riemannian manifold), complex (Kähler structure), algebraic (sphere, Riemannian sphere, torus – elliptic curves – Weierstrass elliptic functions). [2]

Sixteen points on the Poincaré sphere results from four points of polar angle and azimuthal angle in case of Poincaré rotator, a polarization modulator, which enable dynamic control over a polarization state by execution an arbitrary rotation on the Poincaré sphere, same with Poincaré sphere on organic stereochemistry. The Poincaré rotor is an SU(2) Lie group operator, with two U(1) operations to change the phase and the

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**Received:** 1 May 2024; **Accepted:** 20 May 2024; **Published:** 3 June 2024



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amplitude of the state, able to achieve distinguishable  $4 \times 4 = 16$ ,  $8 \times 8 = 64$ ,  $10 \times 10 = 100$  states on the Poincaré sphere after modulating both the phase and amplitude. The molecular structure of Buckminsterfullerene (C<sub>60</sub>) was drawn using the polarization states on the sphere. [3] Geometrical consideration of Stokes parameters on the Poincaré sphere, relationship for parametrization of ellipse based on angle orientation and ellipticity. The wave function corresponds to a point on a surface of a unit sphere R in 4-dimensions, isomorphic to a complex unit sphere C in 2-dimension. A point on a surface of a hypersphere described a state of coherent photons in quantum wave function. [4]

Lie N-algebra is a N-manifold having homological vector field. [5] N-Sphere having (N+1) dimensional Euclidean Space. Topological Poincaré conjecture is a 4-manifold, 1 torus is a circle and a square flat torus is a 3-sphere  $S^3$ . Poincaré group is a 10 dimensional Lie group of affine isometries of the Minkowski space. Minkowski space closely associated but different with Einstein's theories of special relativity and general relativity, in the Minkowski space the Einstein Universe is approximated at the point of observation with conventional time and energies in the local flat space. Segal replaced the Minkowski space  $M_0$  with unique four dimension manifold M, in fact the Euclidean space  $E^3$  of  $M_0$  is replaced by a sphere  $S^3$  of small but nonvanishing curvature, a deformation of M into  $M_0$ , and  $SU(2,2)$  into the Poincaré group as the formation of the "flat" limit of "curved" picture. [6]

3-Sphere approach for calculation of the dihedral [7] and tetrahedral angles [8-10] from NMR data, having as mathematical theories Hopf fibration and Lie algebra. [11] Manifolds [11] locally in Euclidean space or algebraic can be used for calculation dihedral angles from carbon and/or proton chemical shift or only from vicinal coupling constant  $^3J_{HnHn+1}$  [Hz]. Dihedral angle can be represented on three concentric cones having six dihedral angle and two algebraic angles,  $3 \times \phi_1$  and  $2 \times \phi_2$ , which after translation from 3D to 2D can be represented on two sets angles having as point of linkage half of  $\phi_1$  of sets A and B equal with first angle of set B and A. First angles of sets A and B are equals  $\phi_2$  of sets D and F resulting other four sets angles, totally seven sets angles under U or S rule: a. first angles higher as 5[deg] unit U, b. first angles smaller as 5 [deg] unit S. [11] On six sets angles from two units can be found dihedral angles with all stereochemistry, on 14 sets angles are found in close relationship tetrahedral and dihedral angles: a. seven sets starting with U unit and seven with S unit in case of tetrahedral angles  $\phi_{Cn}$  [deg] of five membered ring calculated from vicinal coupling constant  $^3J_{HnHn+1}$  [Hz], b. under *sin* and *tan* function in case of tetrahedral angles  $\phi_{Cn}$  [deg] of five membered ring calculated from chemical shift  $\Delta\delta_{CnCn+1}$  [ppm]. [8] Recorded NMR data are transformed from ppm in gauss and trans-

formed in angle with manifold equations [11], then with calculated angle are builds units:

$$C_n = U_n^{Ni}, S_n^{Ni}, T_n = U_n^{Ni}, S_n^{Ni},$$

with  $I = 1 - 6$ ,  $n = 1 - 7$ ,  $N = A, B, C, D, E, F$ .

Angle with values almost equals with angle calculated only from vicinal constant coupling will be dihedral angle, its relationship with tetrahedral angle [8-10] can be determined with already published trigonometric equations or following the relationship on 14 sets angles on two units based on  $\theta$  and  $\phi$ .

## 2. Results

### 2.1. Manifolds Java Script Programs

#### 2.1.1. Rectangle Approach

Rectangle approach [12] with its geometrical variation: kite – trapezoid – antiparallelogram – irregular, with non-coplanar line – middle line – antirecatangle middle line, transformed in angles of skew circles (eq. 1-2) and middle circles (eq. 3-4) are used for building units and established the dihedral angle.

*Skew circles:*

$$\theta^{An} = 2x \sqrt{\frac{90x(\Delta\delta_{HnHn+1} \times \Delta\delta_{CnCn+1})}{2}} \text{ [deg]} \quad (1)$$

*cis-ea, -ae, trans-ee*

$$\theta^{An} = \sqrt{\frac{90x(\Delta\delta_{HnHn+1} \times \Delta\delta_{CnCn+1})}{2}} \text{ [deg]} \quad (2)$$

*trans-aa*<sup>6,1</sup>

*Middle circles:*

$$\theta^{An} = 2x \sqrt{\frac{90x(\Delta\delta_{HnHn+1} + \Delta\delta_{CnCn+1})}{2}} \text{ [deg]} \quad (3)$$

*cis-ea, -ae, trans-ee*

$$\theta^{An} = \sqrt{\frac{90x(\Delta\delta_{HnHn+1} - \Delta\delta_{CnCn+1})}{2}} \text{ [deg]} \quad (4)$$

*trans-aa*<sup>6,1</sup>

where:  $\theta^{An}$  –angle of set A from unit U or S,  $\Delta\delta_{HnHn+1}$ ,  $\Delta\delta_{CnCn+1}$  – the differences between two consecutive protons and two atoms of carbon [ppm].

```

<!DOCTYPE html>
<html>
<head>
<title>A Java script including HTML</title>

</head>

<body style="background-color:LightGrey;">

<p id="demo"></p>
<p>Click button to:</p>
<button onclick="window.print()">Print this page.</button>

<button
type="button"onclick="document.getElementById('demo').innerHTML
= Date()">Date and Time.</button>

<h2>Java Script program for calculation dihedral angle with rectangle as
manifold.</h2>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program that predict angles of set A[deg]

var usedataX
usedataX = prompt ("The value of cis vicinal coupling constant[Hz]")
usedataXX = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>cis</i> vicinal coupling constant
<sup>3</sup></sup></p><i>J</i><sub>HH</sub>[Hz]</b>=",usedataX);
document.write("<p><i>Cis</i>-HnHn+1.",usedataXX);

var usedataY
usedataY = prompt ("The value of trans-ee vicinal coupling
constant[Hz]")
usedataYY = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>trans-ee</i> vicinal coupling constant
<sup>3</sup></sup></p><i>J</i><sub>HH</sub>[Hz]</b>=",usedataY);
document.write("<p><i>Trans-ee</i>-HnHn+1.",usedataYY);

var usedataZ
usedataZ = prompt ("The value of trans-aa vicinal constant
coupling[Hz]")
usedataZZ = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>trans-aa</i> vicinal coupling constant
<sup>3</sup></sup></p><i>J</i><sub>HH</sub>[Hz]</b>=",usedataZ);
document.write("<p><i>Trans-aa</i>-HnHn+1.",usedataZZ);

var usedataA
usedataA = prompt ("Value of Cn[ppm]")

var usedataB
usedataB = prompt ("Value of Cn[ppm]")

//calculate the difference in chemical shifts between two atoms of carbon
var CnCm = usedataA - usedataB;//CnCm in ppm

if (CnCm < 0){
var CnCm = usedataB - usedataA;//CnCm in ppm
}
else {
var CnCm = usedataA - usedataB;//CnCm in ppm
}

//calculate MinC[ppm]
var MinC = 1/CnCm;//MinC in 1/ppm

if (CnCm > 1){
var MinC = 1/CnCm;//MinC in 1/ppm
}
else{
var MinC = CnCm//MinC in ppm
}

//calculate MaxC[ppm]
var MaxC = 1/CnCm//MaxC in 1/ppm

if (CnCm < 1){
var MaxC = 1/CnCm//MaxC in 1/ppm
}
else{
var MaxC = CnCm//MaxC in ppm
}

document.write("<h4>Carbon chemical shifts.</h4> ");
document.write("<p>Cn[ppm] type in = ",usedataA);
document.write("<p>Cm[ppm] type in = ",usedataB);
document.write("<p>The difference in chemical shifts between two
atoms of carbon CnCm[ppm] = "+CnCm);
document.write("<p>The difference in chemical shifts between two
atoms of carbon with value smaller as 1, MinC = "+MinC);
document.write("<p>The difference in chemical shifts between two
atoms of carbon with value higher as 1, MaxC = "+MaxC);

var usedata2A
usedata2A = prompt ("Value of Hn[ppm]")
var usedata2B
usedata2B = prompt ("Value of Hm[ppm]")

//calculate the difference in chemical shift between two atoms of carbon
var HnHm = usedata2A - usedata2B//HnHm in ppm

if (HnHm < 0){
var HnHm = usedata2B - usedata2A//HnHm in ppm
}
else {
var HnHm = usedata2A - usedata2B//HnHm in ppm
}

//calculate |HnHm|ppm the inverse of HnHm[ppm]
var |HnHm| = 1/HnHm//|HnHm| in 1/ppm

if (|HnHm| < 1){
var |HnHm| = 1/HnHm//|HnHm| in 1/ppm
}
else{
var |HnHm| = HnHm//|HnHm| in ppm
}

//calculate MinH[ppm]
var MinH = 1/|HnHm|//MinH in 1/ppm

if (HnHm > 1){
var MinH = 1/HnHm//MinH in 1/ppm
}
else{
var MinH = HnHm//MinH in ppm
}

//calculate MaxH[ppm]
var MaxH = 1/HnHm//MaxH in 1/ppm

if (HnHm < 1){
var MaxH = 1/HnHm//MaxH in 1/ppm
}
else{
var MaxH = HnHm//MaxH in ppm
}

document.write("<h4>Proton chemical shift.</h4> ");
document.write("<p>Hn[ppm] type in = ",usedata2A);
document.write("<p>Hm[ppm] type in = ",usedata2B);
document.write("<p>The difference in chemical shifts between two
protons HnHm[ppm] = "+HnHm);
document.write("<p>The difference in chemical shifts between two
protons with value smaller as 1, MinH = "+MinH);
document.write("<p>The difference in chemical shifts between two
protons with value higher as 1, MaxH = "+MaxH);

//calculate the angle U1AQ1 of set A in deg for cis or trans-ee
stereochemistry
var Q1a = 90*[(MaxC*MinH)/2];//calculate Q1a
var Q1b = Math.sqrt(Q1a)/value of Q1b[deg]
var U1AQ1 = 2*Q1b//value of U1AQ1[deg]

document.write("<p><b>Skew line of rectangle</b><: <i>Cis</i> and
<i>trans-ee</i> stereochemistry.</h4>");

document.write("<p><b>Case Ia</b></p> (C*1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis or trans-ee
stereochemistry
var Q1a = 90*[(MinC*MinH)/2];//calculate Q1a
var Q1b = Math.sqrt(Q1a)/value of Q1b[deg]
var U1AQ1 = 2*Q1b//value of U1AQ1[deg]

document.write("<p><b>Case Ib</b></p> (1/C*1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis or trans-ee
stereochemistry
var Q1a = 90*[(MaxC*MaxH)/2];//calculate Q1a
var Q1b = Math.sqrt(Q1a)/value of Q1b[deg]
var U1AQ1 = 2*Q1b//value of U1AQ1[deg]

document.write("<p><b>Case Ic</b></p> (C*H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MinC + MinH)/2];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 2*Q1d//value of U1AQ1[deg]

document.write("<p><b>Middle line of rectangle</b></p>");
document.write("<p><b>Case IIa</b></p> (1/C + 1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MaxC + MinH)/2];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 2*Q1d//value of U1AQ1[deg]

document.write("<p><b>Case IIb</b></p> (1/C + 1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MinC - MinH)/2];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 2*Q1d//value of U1AQ1[deg]

document.write("<p><b>Middle line of antiparalelogram</b>");
document.write("<p><b>Case IIIa</b></p> (1/C - 1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MaxC - MinH)/2];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 2*Q1d//value of U1AQ1[deg]

document.write("<p><b>Case IIId</b></p> (C - 1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MinC - MinH)/1];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 1*Q1d//value of U1AQ1[deg]

document.write("<p><b>Case IIIc</b></p> (1/C - 1/H, m = 1): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for cis stereochemistry
var Q1c = 90*[(MaxC - MinH)/1];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 1*Q1d//value of U1AQ1[deg]

document.write("<p><b>Case IIId</b></p> (C - 1/H, m = 1): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for trans-aa stereochemistry
var Q1a = 90*[(MaxC*MinH)/2];//calculate Q1a
var Q1b = Math.sqrt(Q1a)/value of Q1b[deg]
var U1AQ1 = 1*Q1b//value of U1AQ1[deg]

document.write("<h4><b>Skew line of rectangle</b><: <i>Trans-aa</i>
stereochemistry.</h4>");
document.write("<p><b>Case IV</b></p> (C*(1/H)): angle U1AQ1[deg] =
"+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for trans-aa stereochemistry
var Q1c = 90*[(MinC + MinH)/2];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 2*Q1d//value of U1AQ1[deg]

document.write("<h4><b>Middle line of rectangle</b><: <i>Trans-
aa</i> stereochemistry.</h4>");
document.write("<p><b>Case Va</b></p> (1/C + 1/H, m = 2): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for trans-aa stereochemistry
var Q1c = 90*[(MinC - MinH)/1];//calculate Q1c
var Q1d = Math.sqrt(Q1c)/value of Q1d[deg]
var U1AQ1 = 1*Q1d//value of U1AQ1[deg]

document.write("<p><b>Case Vb</b></p> (1/C + 1/H, m = 1): angle
U1AQ1[deg] = "+U1AQ1);

//calculate the angle U1AQ1 of set A in deg for trans-aa stereochemistry
with 3JHH higher as 9.5[Hz]
var Q1a = 90*[(MaxC*MaxH)/2];//calculate Q1a
var Q1b = Math.sqrt(Q1a)/value of Q1b[deg]
var U1AQ1 = 1*Q1b//value of U1AQ1[deg]

document.write("<h4>VI: <i>Trans-aa</i> stereochemistry with
<sup>3</sup></sup></p><i>J</i><sub>HH</sub> higher as 9.5[Hz]</h4>");
document.write("<p><b>Case VI</b></p> (C*H): angle U1AQ1[deg] =
"+U1AQ1);

alert("Hello World!");

```

**Figure 1.** Java Script program ScienceRectangle.html for calculation of dihedral angles with rectangle eq. 1-4 from chemical shift  $\delta$ [ppm].

As observation: instead of n used for *cis* and *trans* stereochemistry in case of Skew and Middle circles can be applied the rule used for calculation of the vicinal coupling constant

$^3J_{\text{HnHn+1}}$ [Hz] from vicinal angle  $\phi$ [deg] (eq. 5-8).

$$\text{Trans: } ^3J_{\text{HH}} = \sqrt{\phi} \quad (5)$$



$$\text{Cis: } {}^3J_{\text{HH}} = \frac{\sqrt{\Phi}}{2} \quad (6)$$

$$\theta^{\text{An}} = \sqrt{A}, \quad A = f(\Delta\delta_{\text{HnHn+1}}, \Delta\delta_{\text{CnCn+1}}) \quad (7)$$

$$\theta^{\text{An}} = \frac{\sqrt{A}}{2}, \quad A = f(\Delta\delta_{\text{HnHn+1}}, \Delta\delta_{\text{CnCn+1}}) \quad (8)$$

Java Script program presented at ACS spring 2021 for calculation of the dihedral angles from carbon and proton chemical shift  $\delta_{\text{Cn}}[\text{ppm}]$  with rectangle equations in 3 steps [13]: 1. Prediction of de dihedral angles  $\theta_{\text{HnHn+1}}[\text{deg}]$  only from vicinal coupling constants  ${}^3J_{\text{HnHn+1}}[\text{Hz}]$  without torus inversion; 2. Calculation the first angle of set B or half  $\phi_1$  of set A; 3. Building three sets angles for all equations (eq. 1-4),

### 2.1.2. Cyclide Approach

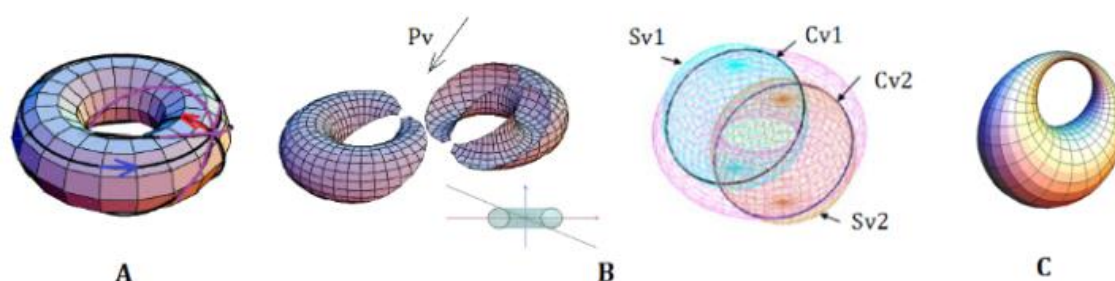


Figure 2. Torus (A) and Dupin Cyclide (C).

A. Villarceau circles Cv1 and Cv2, or two sphere Sv1 and Sv2 result at intersection with a bitangent plane Pv, which meet all of the parallel circular cross-sections of the torus at the same angle (Figure 2). [14, 15]

$$\theta_{\text{T}}^{\text{NA}} = \sin^{-1}\left(\frac{\Delta\delta_{\text{HH}}}{\Delta\delta_{\text{CC}}}\right) \quad (9)$$

$$\theta_{\text{T}}^{\text{NB}} = \cos^{-1}\left(\frac{\Delta\delta_{\text{HH}}}{\Delta\delta_{\text{CC}}}\right) \quad (10)$$

$$\theta_{\text{D}}^{\text{NA}} = \tan^{-1}\left(\frac{\Delta\delta_{\text{HH}}}{\Delta\delta_{\text{CC}}}\right) \quad (11)$$

$$\theta_{\text{D}}^{\text{NB}} = \cotan^{-1}\left(\frac{\Delta\delta_{\text{HH}}}{\Delta\delta_{\text{CC}}}\right) \quad (12)$$

Where:  $\Delta\delta_{\text{HnHn+1}}$ ,  $\Delta\delta_{\text{CnCn+1}}$  – the differences between two consecutive protons and two atoms of carbon [ppm],  $\theta_{\text{T}}^{\text{NA, NB}}$ ,  $\theta_{\text{D}}^{\text{NA, NB}}$  – Villarceau circles of torus and Dupin cyclide.

B. Dupin cyclide non-spherical algebraic surface of degree four, compatible with inversion of torus, having embedded all four characteristics circles of torus (Figure 2). [14, 15]

Torus equations for calculation one characteristic angle of first set in function of the physical transformation reveals that

and choosing of the dihedral angle with values almost equals with angles calculated only from vicinal coupling constant. If the required dihedral angle is not found on unit with three sets angles can be used the program for transformation from U to S and *viceversa*, [11] also can be calculated the vicinal coupling constant from the calculated dihedral angle. [14]

In figure 1 is presented Java Script program ScienceRectangle.html for calculation of the dihedral angles from carbon and proton chemical shift [11] with rectangle eq. 1-4, in fact only one angle of set A. Then with this angle are build units with seven sets angles and analyzed the stereochemistry and the sign of dihedral angle. The program for prediction was improved to date. [7]

the proton and carbon chemical shifts transformed in gauss don't fit into the Hopf fibration relationship between three sets angles, instead using the transformation on Hz the units can be built in line with Hopf fibration rule. A. Transformation in Hz [15]:

$$\theta_{\text{W}}^{\text{NA}} = \sin^{-1}(\Delta\delta_{\text{HnHn+1}}\omega_{\text{H}}/\Delta\delta_{\text{CnCn+1}}\omega_{\text{C}}) \quad (13)$$

$$\text{Euler character: } \sin\theta_{\text{WE}}^{\text{A}} = \cos\theta_{\text{WE}}^{\text{B}} \quad (14)$$

B. Transformation in gauss:

$$\theta_{\text{W}}^{\text{NA}} = \sin^{-1}(\Delta\delta_{\text{HnHn+1}}\omega_{\text{H}}/\gamma_{\text{H}}/\Delta\delta_{\text{CnCn+1}}\omega_{\text{C}}/\gamma_{\text{C}}) \quad (15)$$

$$\text{Without Euler character: } \sin\theta_{\text{WF}}^{\text{A}} \neq \cos\theta_{\text{WF}}^{\text{B}} \quad (16)$$

Where:  $\Delta\delta_{\text{HnHn+1}}$ ,  $\Delta\delta_{\text{CnCn+1}}$  – the differences between two consecutive protons and two atoms of carbon [ppm],  $\omega_{\text{L}}$  – Larmor frequency [ ${}^{13}\text{C}$ : 75MHz,  ${}^1\text{H}$  400MHz],  $\nu$  – frequency [Hz],  $\delta$  – chemical shifts [ppm],  $\gamma$  – gyromagnetic ratio:  ${}^{13}\text{C}$ :  $\gamma = 10.71 [\text{MHzxT}^{-1}] = 6.7[10^7\text{radxT}^{-1}\text{xs}^{-1}]$ ,  ${}^1\text{H}$ :  $\gamma = 42.57 [\text{MHzxT}^{-1}] = 26.7[10^7\text{radxT}^{-1}\text{xs}^{-1}]$ .

```

<!DOCTYPE html>
<html>
<head>
<title>A Java script including HTML</title>

</head>

<body style="background-color:LightGrey;">

<p id="demo"></p>
<p>Click button to:</p>
<button onclick = "window.print()">Print this page.</button>

<button
type="button"onclick="document.getElementById('demo').innerHTML
= Date()">Date and Time.</button>

<h3>Java Script program for calculation dihedral angle from NMR data
with Villarceau circles.</h3>

</body>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program that predict and calculated dihedral angles[deg]

var usedata1A
usedata1A = prompt ("The value of cis vicinal coupling constant[Hz]")
usedataA = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>cis</i> vicinal coupling constant
<sup>3</sup></sup><i>J</i></sub>HH</sub>[Hz]</b>=",usedata1A)

document.write("<p><i>cis</i>-HnHn+1:",usedataA)

var usedata2B
usedata2B = prompt ("The value of trans-ee vicinal coupling
constant[Hz]")
usedataB = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>trans-ee</i> vicinal coupling constant
<sup>3</sup></sup><i>J</i></sub>HH</sub>[Hz]</b>=",usedata2B)
document.write("<p><i>Trans-ee</i>-HnHn+1:",usedataB)

var usedata3C
usedata3C = prompt ("The value of trans-aa vicinal constant
coupling [Hz]")
usedataC = prompt ("The number of protons HnHn+1")

document.write("<p><b>The <i>trans-aa</i> vicinal coupling constant
<sup>3</sup></sup><i>J</i></sub>HH</sub>[Hz]</b>=",usedata3C)
document.write("<p><i>Trans-aa</i> HnHn+1:",usedataC)

var usedata4a
usedata4a = prompt ("Value of Hn[ppm]")
var usedata4b
usedata4b = prompt ("Value of Hm[ppm]")

//calculate the value of HnHm[ppm]
var HnHm = usedata4a - usedata4b;//the differences between two
protons in ppm

if (HnHm < 0){
var HnHm = usedata4b - usedata4a;//the differences between two
protons in ppm
}
else{
var HnHm = usedata4a - usedata4b;//the differences between two
protons in ppm
}

var usedata5
usedata5 = prompt ("1H Larmor frequency [MHz]")

//calculate the value of RmHnHm in [Hz]
var RmHnHm = (HnHm*usedata5);//value of RmHnHm[Hz]

var usedata6a
usedata6a = prompt ("Value of Cn[ppm]")
var usedata6b
usedata6b = prompt ("Value of Cm[ppm]")

//calculate the value of CnCm[ppm]
var CnCm = usedata6a - usedata6b

if (CnCm < 0){
var CnCm = usedata6b - usedata6a;
}
else{
var CnCm = usedata6a - usedata6b;
}

var usedata7
usedata7 = prompt ("13C Larmor frequency [MHz]")

//calculate the value of RmCnCm[Hz]
var RmCnCm = (CnCm*usedata7);//value of RmCnCm[Hz]

//calculate the ratio
var R = RmHnHm/RmCnCm;//ratio proton/carbon

//calculate angle of set U1A1S[deg]
var AS = Math.asin(R);//angle of set AS[rad]
var U1A1S = AS*57.29577521;//angle of set U1A1S[deg]

//calculate angle of set U1A1T[deg]
var AT = Math.atan(R);//angle of set AT[rad]
var U1A1T = AT*57.29577521;//angle of set U1A1T[deg]

document.write("<h4><i>Program for calculation the angle
A1.</i></h4>")
document.write("<p>The Hn[ppm] type in=",usedata4a);
document.write("<p>The Hm[ppm] type in=",usedata4b);
document.write("<p>1H Larmor frequency [MHz] type in=",usedata5);
document.write("<p>The value of HnHm[ppm] is="+HnHm);
document.write("<p>The value of RmHnHm [Hz] is="+RmHnHm);
document.write("<p>The Cn[ppm] type in=",usedata6a);
document.write("<p>The Cm[ppm] type in=",usedata6b);
document.write("<p>13C Larmor frequency [MHz] type type
in=",usedata7);
document.write("<p>The value of CnCm[ppm] is="+CnCm);
document.write("<p>The value of RmCnCm[Hz] is="+RmCnCm);
document.write("<p>The value of R is="+R);
document.write("<p>The angle of set U1A1S[deg] is="+U1A1S);
document.write("<p>The angle of set U1A1T[deg] is="+U1A1T);

alert("Hello World!");
</script>
</html>

```

**Figure 3.** Java Script program ScienceVillarceau.html for calculation of dihedral angles with Cyclide approach from chemical shift  $\delta$ [ppm] with eq. 9-12.

```

<DOCTYPE html>
<html>
<head>
<title>A Java script including HTML </title>

<head>

<body style = "background-color: LightGrey;">

<p style = "font-size: 18px;" id = "demo"><p>
<p style = "font-size: 18px;">Click button to:<p>
<button onclick = "window.print()">Print this page.</button>

<button type="button"
onclick="document.getElementById('demo').innerHTML = Date()">
Date and Time.</button>

<h3>Java Script program for calculation of dihedral angle with polar
equations.</h3>

<h4>Calculation of the dihedral angle from chemical shift and vicinal coupling
constant.</h4>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program that calculate angles of set A[deg]

var usedata1
usedata1 = prompt ("The value of cis or trans-ee vicinal coupling constant[Hz]")
usedataA = prompt ("The number of protons HnHn+1")

document.write("<p><b><i>Cis or trans-ee</i> vicinal coupling constant
<sup>3</sup></sup></b><i>J</i><sub>HH</sub>[Hz]<b>=", usedata1)
document.write("<p><b><i>Cis or trans-ee</i> HnHn+1:", usedataA)

var usedata2
usedata2 = prompt ("The value of trans-aa vicinal constant coupling[Hz]")

usedataB = prompt ("The number of protons HnHn+1")

document.write("<p><b><i>Trans-aa</i> vicinal coupling constant
<sup>3</sup></sup></b><i>J</i><sub>HH</sub>[Hz]<b>=", usedata2)
document.write("<p><b><i>Trans-aa</i> HnHn+1:", usedataB)

var usedata3
usedata3 = prompt ("Value of Xn[ppm], with X = C or H")
var usedata4
usedata4 = prompt ("Value of Xm[ppm], with X = C or H")

//calculate the value of XnXm[ppm]
var XnXm = usedata3 - usedata4

if (XnXm < 0){
var XnXm = usedata4 - usedata3;
}
else {
var XnXm = usedata3 - usedata4;
}

document.write("<h4>Calculation the differences in chemical shift.</h4>")
document.write("<p>The Xn[ppm] =", usedata3);
document.write("<p>The Xn[ppm] =", usedata4);
document.write("<p>The value of XnXm[ppm] =", XnXm);

var usedata5
usedata5 = XnXm/usedata1;//calculate the value of Rc/c
var Rc/c = usedata5;//value of Rc/c

//calculate the angle of set A[deg] for cis or trans-ee stereochemistry
var Rc/c = usedata5;//value of Rc/c
if (Rc/c < 1){
//calculate angle Rc/c in deg
var Rc/c = usedata5;//value of Rc/c
}
else {
var Rc/c = 1/usedata5;//value of Rc/c
}

var Rc = Math.asin(Rc/c);//the dihedral angle Rc[rad] with cis or trans-ee
stereochemistry
var Rcd = (Rc)*57.29577521;//the dihedral angle Rcd[deg] with cis or trans-ee
stereochemistry

//calculate the angle of set A[deg] for cis stereochemistry
var C/c = Rc/c;// value of C/c

if (Rc/c < 1){
//calculate angle C/c in deg for cis stereochemistry
var C/c = 1/Rc/c//angle C/c[deg]
}
else {
var C/c = Rc/c//angle C/c[deg]
}

var D/c = 10*Rc/c// value of D/c

var A/Jcs = (2*C/c)// value of A/Jcs
var A/Jcf = A/Jcs*A/Jcs// value of A/Jcf[deg]

var B/Jcs = (2*D/c)// value of B/Jcs
var B/Jcf = (B/Jcs*B/Jcs)// value of B/Jcf[deg]

//calculate angles with trans-ee stereochemistry
var C/c = Rc/c// value of C/c

if (Rc/c > 1){
//calculate angle C/c in deg for trans-ee stereochemistry
var C/c = 1/Rc/c//angle C/c[deg]
}
else {
var C/c = Rc/c//angle C/c[deg]
}

var D/c = 10*Rc/c// value of D/c

var A/Jes = (2*C/c)// value of A/Jes
var A/Jef = A/Jes*A/Jes// value of A/Jef[deg]

var B/Jes = (2*D/c)// value of B/Jes
var B/Jef = (B/Jes*B/Jes)// value of B/Jef[deg]

document.write("<p><b><i>Cis or trans-ee stereochemistry</i>.</p>");

document.write("<p><b><i>A. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>B. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>C. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>D. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>E. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>F. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>G. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>H. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>I. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>J. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>K. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>L. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>M. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>N. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>O. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>P. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>Q. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>R. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>S. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>T. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>U. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>V. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>W. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>X. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>Y. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>Z. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AA. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AB. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AC. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AD. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AE. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AF. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AG. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AH. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AI. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AJ. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AK. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AL. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AM. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AN. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AO. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AP. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AQ. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AR. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AS. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AT. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AU. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AV. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AW. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AX. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AY. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>AZ. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BA. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BB. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BC. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BD. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BE. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BF. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BG. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BH. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BI. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BJ. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BK. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BL. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BM. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BN. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BO. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BP. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BQ. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BR. Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><b><i>BS. Transformation under stereochemistry and unit
rule</i>.</p&gt
```

**Figure 4.** Java Script program SciencePOLAReq.html for calculation of dihedral angles with polar equations 17-20 from carbon chemical shift  $\delta$ [ppm].

Java Script program ScienceVillarceau.html presented in Figure 3 for calculation of the dihedral angles from carbon and proton chemical shift with cyclide equations (eq. 9-12) start with introduction of the vicinal coupling constant, proton and carbon chemical shift, [11] calculation one angle of set A with eq. 9, 11. A program for calculation of the dihedral angles only from torus Villarceau (eq. 9) circles containing also the step for building of the unit with seven set angle was published. [11]

### 2.1.3. Polar Equations Approach

Polar equations without (eq. 17, 18) or under stereochemistry rule (eq. 19, 20) and homotopic approach (continues transformation from torus to rectangle, from  $\pi$  to  $\text{deg}$ ) are proposed for calculation of dihedral angles  $\theta_{\text{HnHn+1}}[\text{deg}]$  from the ratio differences in chemical shift between two protons or atoms of carbon and vicinal coupling constant  ${}^3J_{\text{HnHn+1}}[\text{Hz}]$ . [16] A ratio used in literature for transformation of the differences in chemical shift between two atoms of carbon from ppm in Hz at values higher as 10, and  $\Delta\nu = J_X(3)^{1/2}$  at smaller

differences of two protons chemical shift, in other words from AB to AX coupling. [17]

$$R_{mH} = \Delta\delta_{HnHn+1}/^3J_{HnHn+1}[s] \quad (17)$$

$$R_{mC} = \Delta\delta_{CnC_{n+1}}/\beta J_{H_nH_{n+1}}[s] \quad (18)$$

Where  $x = C, H$ ,  $R_{mx} = 1/R_{mx}$  or  $R_m = 10xR_{mx}$

$$cis, trans-ee: (2xR_{mH})^2 = \theta_x \quad (19)$$

$$trans-aa: (R_{mH})^2 = \theta_x \quad (20)$$

$$(v_4 - v_1)/(v_3 - v_2) = \tan^2\theta \quad (21)$$

$$(v_1 - v_3) = (v_2 - v_4) = (\Delta v^2 + J^2)^{1/2} \quad (22)$$

Where  $v_n - n = 1 - 4$ , four pics of the two coupled protons.

```

<!DOCTYPE html>
<html>
<head>
<title>A Java script including HTML</title>

</head>

<body style="background-color:LightGrey;">

<p id="demo"></p>
<p>Click button to:</p>
<button onclick = "window.print()">Print this page.</button>

<button
type="button"onclick="document.getElementById('demo').innerHTML
= Date()">Date and Time.</button>

<h3>Java Script program for calculation dihedral angle with Euler-
Conic approach from chemical shift.</h3>

</body>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program that predict and calculate dihedral angles

var usedata1 a
usedata1 a = prompt ("Value of Hn[ppm]")
var usedata1 b
usedata1 b = prompt ("Value of Hm[ppm]")

//calculate the value of CnCm[ppm]

var HnHm = usedata1 a - usedata1 b;//the differences between two
protons in ppm

if (HnHm < 0){
var HnHm = usedata1 b - usedata1 a;//the differences between two
protons in ppm
}
else{
var HnHm = usedata1 a - usedata1 b;//the differences between two
protons in ppm
}

var usedata2
usedata2 = prompt ("1H Larmor frequency [MHz]")

//calculate the value of RmH in [gauss]
var RmH = (4*HnHm*usedata2)/(42.57*1000);//value of RmH[gauss]

//calculate the angle of set Ai in rad
var ArH = Math.asin(RmH);// value of set ArH[rad]

//calculate the angle of set A1 in deg
var U1Ah1 = ArH*57.29577521;// value of set U1Ah1[deg]

//calculate the angle of set Bi in rad
var BrH = Math.acos(RmH);// value of set BrH[rad]

//calculate the angle of set B1 in deg
var U1Bh1 = BrH*57.29577521;// value of set U1Bh1[deg]

document.write("<h4><i>Program for calculation the dihedral angle
from proton chemical shift.</i></h4>")

document.write("<p>1H Hn[ppm] type in=",usedata1 a);
document.write("<p>The Hm[ppm] type in=",usedata1 b);
document.write("<p>1H Larmor frequency [MHz] type in=",usedata2);
document.write("<p>The value of HnHm[ppm] is="+HnHm);
document.write("<p>The value of RmH[gauss] is="+RmH);
document.write("<p>The angle U1Ah1[deg] is="+U1Ah1);
document.write("<p>The angle U1Bh1[deg] is="+U1Bh1);

var usedata3 a
usedata3 a = prompt ("Value of Cn[ppm]")
var usedata3 b
usedata3 b = prompt ("Value of Cm[ppm]")

//calculate the value of CnCm[ppm]
var CnCm = usedata3 a - usedata3 b

if (CnCm < 0){
var CnCm = usedata3 b - usedata3 a;
}
else{
var CnCm = usedata3 a - usedata3 b;
}

var usedata4
usedata4 = prompt ("13C Larmor frequency [MHz]")

//calculate the value of RmC in [gauss]
var RmC = (4*CnCm*usedata4)/(10.71*1000);//value of RmC[gauss]

//calculate the angle of set Ai in rad
var ArC = Math.asin(RmC);// value of set ArC[rad]

//calculate the angle of set A1 in deg
var U1Ac1 = ArC*57.29577521;// value of set A1[deg]

//calculate the angle of set Bi in rad
var BrC = Math.acos(RmC);// value of set BrC[rad]

//calculate the angle of set B1 in deg
var U1Bc1 = BrC*57.29577521;// value of set B1[deg]

document.write("<h4><i>Program for calculation the dihedral angle
from carbon chemical shift.</i></h4>")

document.write("<p>The Cn[ppm] type in=",usedata3a);
document.write("<p>The Cm[ppm] type in=",usedata3b);
document.write("<p>13C Larmor frequency [MHz] type
in=",usedata4);
document.write("<p>The value of CnCm[ppm] is="+CnCm);
document.write("<p>The value of RmC[gauss] is="+RmC);
document.write("<p>The angle U1Ac1[deg] is="+U1Ac1);
document.write("<p>The angle U1Bc1[deg] is="+U1Bc1);

alert("Hello World!");
</script>
</html>

```

**Figure 5.** Java Script program EulerConic.html for calculation of dihedral angles with Euler-Conic approach with eq. 23.

#### 2.1.4. Euler-Conic Approach

One angle of first set can be calculated from the differences in chemical shift between two protons  $\Delta\delta_{HnHn+1}$ [ppm] or two atoms of carbons  $\Delta\delta_{CnCn+1}$ [ppm] with Euler-Conic equation 23. [11]

$$\theta = \sin^{-1}R_{mx}[\text{deg}] \quad (23)$$

Where  $R_{mx} = \Delta\delta_{XnXn+1}\omega_H/4\pi \times 10^{-3}/\gamma_H$  [gauss],  $x = C, H$ ;  $\Delta\delta_{XnXn+1}$  – the differences between two consecutive protons and two atoms of carbon [ppm],  $\omega_L$  – Larmor frequency [ $^{13}\text{C}$ : 75MHz,  $^1\text{H}$  400MHz],  $\nu$  – frequency [Hz],  $\delta$  – chemical shifts [ppm],  $\gamma$  – gyromagnetic ratio.



```

<DOCTYPE html>
<html>
<head>
<title>A Java script including HTML</title>

</head>

<body style = "background-color:LightGrey;">

<p id = "demo"><p>
<p>Click button to<p>
<button onclick = "window.print()">Print this page<button>

<button
type="button"onclick="document.getElementById(demo).innerHTML
= Date()">Date and Time<button>

</>JavaScript program for calculation dihedral angle from NMR data
with Villacium circles</>

</body>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program that predict and calculated dihedral angles[deg]

var usdata1A
usdata1A = prompt ("The value of cis vicinal coupling constant[Hz]")
usdata1A = prompt ("The number of protons Hn(n=1)")

document.write("<p><b>The</b><b>cis</b><b> vicinal coupling constant
<sup>3</sup><sub>H</sub><sup>1</sup><sub>H</sub>[Hz]<b>:"<b>usdata1A)

document.write("<p><b>cis</b><b>Hn(n=1, usdata1A)

var usdata2B
usdata2B = prompt ("The value of trans vicinal coupling
constant[Hz]")
usdata2B = prompt ("The number of protons Hn(n=1)")

document.write("<p><b>The</b><b>trans</b><b> vicinal coupling constant
<sup>3</sup><sub>H</sub><sup>1</sup><sub>H</sub>[Hz]<b>:"<b>usdata2B)
document.write("<p><b>trans</b><b>Hn(n=1, usdata2B)

var usdata3C
usdata3C = prompt ("The value of trans-aa vicinal constant
coupling[Hz]")
usdata3C = prompt ("The number of protons Hn(n=1)")

document.write("<p><b>The</b><b>trans-aa</b><b> vicinal coupling constant
<sup>3</sup><sub>H</sub><sup>1</sup><sub>H</sub>[Hz]<b>:"<b>usdata3C)
document.write("<p><b>trans-aa</b><b>Hn(n=1, usdata3C)

var usdata4a
usdata4a = prompt ("Value of Ha[ppm]")
var usdata4b = prompt ("Value of Hb[ppm]")

//calculate the value of HnHm[ppm]
var HnHm = usdata4a - usdata4b//the differences between two
protons in ppm

if (HnHm < 0){
var HnHm = usdata4b - usdata4a//the differences between two
protons in ppm
}
else{
var HnHm = usdata4a - usdata4b//the differences between two
protons in ppm
}

var usdata5
usdata5 = prompt ("1H Larmor frequency [MHz]")

//calculate the value of RnHnHm in [Hz]
var RnHnHm = (HnHm*usdata5)/value of RnHnHm[Hz]

var usdata6a
usdata6a = prompt ("Value of Cn[ppm]")
var usdata6b = prompt ("Value of Cn[ppm]")

//calculate the value of CnCm[ppm]
var CnCm = usdata6a - usdata6b

if (CnCm < 0){
var CnCm = usdata6b - usdata6a;
}
else{
var CnCm = usdata6a - usdata6b;
}

var usdata7
usdata7 = prompt ("13C Larmor frequency [MHz]")

//calculate the value of RnCnCm[Hz]
var RnCnCm = (CnCm*usdata7)/value of RnCnCm[Hz]

</DOCTYPE html>
</html>
</head>
<title>A Java script including HTML</title>

</head>

<body style = "background-color:LightGrey;">

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<p>Click button to<p>
<button onclick = "window.print()">Print this page<button>

<button
type="button"onclick="document.getElementById(demo).innerHTML
= Date()">Date and Time<button>

</>JavaScript program for calculation dihedral angle from NMR data
with 3-sphere approach</>

</body>

<script type="text/javascript">
//File name Dihedral angle [deg].html
//Program for calculation seven sets angles [deg]

var usdata1
usdata1 = prompt ("The value of A[deg]")
var A = usdata1/angle A[deg]
//calculate angle A1[deg]

var A1 = 1*A/angle A1[deg]

document.write("<b><b>Building seven sets units</b>:"<b>);

document.write("<p>Angle A1[deg]:"<b>A1);

var usdata2
usdata2 = A1//The value of half A1[deg]
var A1 = usdata2/angle A1[deg]

//calculate angles of set A1 in deg
var A1 = (A1, A2, A3, A4, A5, A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, A20, A21, A22, A23, A24, A25, A26, A27, A28, A29, A30, A31, A32, A33, A34, A35, A36, A37, A38, A39, A40, A41, A42, A43, A44, A45, A46, A47, A48, A49, A50, A51, A52, A53, A54, A55, A56, A57, A58, A59, A60, A61, A62, A63, A64, A65, A66, A67, A68, A69, A70, A71, A72, A73, A74, A75, A76, A77, A78, A79, A80, A81, A82, A83, A84, A85, A86, A87, A88, A89, A90, A91, A92, A93, A94, A95, A96, A97, A98, A99, A100, A101, A102, A103, A104, A105, A106, A107, A108, A109, A110, A111, A112, A113, A114, A115, A116, A117, A118, A119, A120, A121, A122, A123, A124, A125, A126, A127, A128, A129, A130, A131, A132, A133, A134, A135, A136, A137, A138, A139, A140, A141, A142, A143, A144, A145, A146, A147, A148, A149, A150, A151, A152, A153, A154, A155, A156, A157, A158, A159, A160, A161, A162, A163, A164, A165, A166, A167, A168, A169, A170, A171, A172, A173, A174, A175, A176, A177, A178, A179, A180, A181, A182, A183, 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protons leads to difference in system of equations [17], thus on the unit are found in function of the values of coupling constant different equation: the transformation from U to S through first angle of set  $\theta^{UB1}$  leading to third angles of set  $\theta^{SA3}$  with eq. 24.

$$\theta^{SB3} = nx(3x\theta^{UB1}), n = 1, 2 \quad (24)$$

Where:  $\theta^{UB1}$  – first angle of set B from unit U ( $\theta^{N1} > 5[\text{deg}]$ ),  $\theta^{SB3}$  – third angle of set B from unit S ( $\theta^{N1} < 5[\text{deg}]$ ),  $N = A, B, C, D, E, F, G$ .

## 2.2. Seven Sets Unit

Seven sets angles, three Venn diagrams A, B, C - D, E, A - F, G, B, with angles between 69 - 70[deg] in case of unit U1, and with angles between 60 - 65[deg] in case of unit S1, or two units U1 and one S1 and *vice-versa*, can be calculated with Java Script program ScienceSevenUnit.html (Figure 6).

$$U1 = U1Ai, U1Bi, U1Ci, U1Di, U1Ei, U1Fi, U1Gi$$

Where:  $U1A1 > 5[\text{deg}]$ ,  $S1A1 < 5[\text{deg}]$ ,  $i = 1-6$ .

## 3. Discussion

The Java Script programs presented for calculation from chemical shift  $\delta[\text{ppm}]$  and/or vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  enable a carefully analysis of dihedral angles  $\theta_{\text{HnHn+1}}[\text{deg}]$  with corresponding sign and stereochemistry. Since bond distances  $l_{\text{CnCn+1}}[\text{\AA}]$  between two atoms of carbon are all under different polar equations (*i.e.* limaçons or cardioid, rose or lemniscate) our expectation was to find different equations for calculation the best angle, much more the differences between dihedral angles calculated from carbon and proton chemical shift and vicinal coupling constant with varies manifolds to give information about the limits of deviation from planarity.

Dihedral angles calculated with Rectangle approach (eq. 1-4) and Java Script ScienceRectangle.html program from carbon and proton chemical shift are published to date, and results are remarkable. [12]

Eular-Conic approach (eq. 23) for calculation of the dihedral angles from carbon or proton chemical shift with Java

Script program EulerConic.html is probable the preferred one. [11] Because smaller differences are observed in case of iminocyclitols studied to date between unit builds from *sin* and *tan* functions, in Java Script program presented in Figure 5 are calculated only *sin* and *cos* functions, angles of set A and B. Units calculated from *sin* and *tan* functions are used for calculation of the dihedral  $\theta_{\text{HnHn+1}}[\text{deg}]$  and tetrahedral angles  $\phi_{\text{Cn}}[\text{deg}]$  in opposite. [8]

Villarceau approach (eq. 9-12) and Java Script program ScienceVillarceau.html (Figure 3) enable calculation of the dihedral angles  $\theta_{\text{HnHn+1}}[\text{deg}]$  from the ratio proton/carbon chemicals shift  $\delta[\text{ppm}]$  transformed in Hz, since gauss transformation don't give the expected correlation between set A and set B, resulting two seven set units. Along the *sin* function [11] in this paper was introduced the *tan* function, in attempt to find the almost equals values between recorded and calculated vicinal coupling constant. In case of isopropylidene protected iminocyclitol 1 [18] (Figure 7) for a vicinal coupling constant of 5.4[Hz] was calculated from *tan* function a vicinal coupling constant of 5.4[Hz] relative to 5.37[Hz] calculated from *sin* function.

$$\text{Trans-ee: } \theta_{\text{H3H4}} = \tan^{-1}(\sin-\phi) \quad (25)$$

$$\text{Trans-ee: } \theta_{\text{H3H4}} = \sin^{-1}(\tan-\phi) \quad (26)$$

Dihedral angles are calculated with Java Script SciencePolareq.html (Figure 4) and polar equations approach eq. 17-20 from the differences between two protons chemical shift  $\Delta\delta_{\text{HnHn+1}}[\text{ppm}]$  or two carbons chemical shift  $\Delta\delta_{\text{CnCn+1}}[\text{ppm}]$  and vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  (Tables 1 and 2), using once the *sin* and *cos* function and second the homotopic approach [19]. In second case are calculated angles with and without vicinal angle rule ( $\theta^A$ ,  $\theta_X^A[\text{deg}]$ ). All the programs presented gives one or two angles of first and second sets angles A and B, angles used for building seven sets unit and chose the dihedral angle with value almost equal with dihedral angle  $\theta_{\text{HnHn+1}}[\text{deg}]$  calculated only from vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  In accord with D-ribitol stereochemistry, iminocyclitols 1-3 [18] (Figure 7) have negative dihedral angle  $\theta_{\text{H3H4}}[\text{deg}]$ , angle calculated with equations 25, 26.

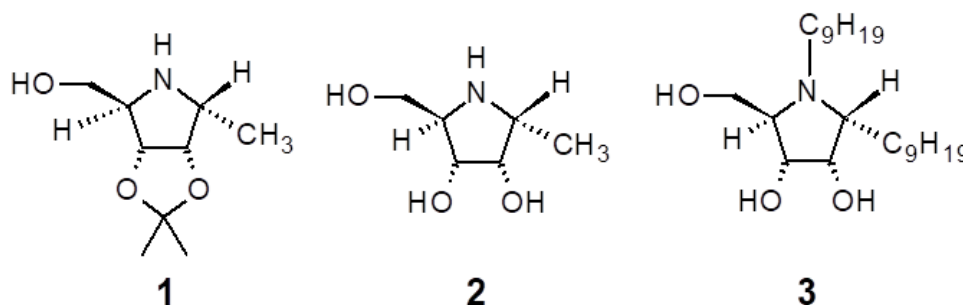


Figure 7. Iminocyclitols 1-3 with  $C_1$ -R- $\alpha$ -Dribitol stereochemistry [18].

**Table 1.** Dihedral angles of iminocyclitols 1-3 calculated from differences between chemical shift  $\Delta\delta_{\text{Hn}}[\text{Hz}]$  of two protons and vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  with polar equations 17, 19, 20.

Entry	$^3J_{\text{HH}}^{\text{a}} [\text{Hz}]$	$H_n [\text{ppm}]$	$R_{\text{mH}} [\pi]$	$\theta [\text{deg}], ^3J_{\text{HH}} [\text{Hz}]$	$\theta^{\text{A}} [\text{deg}]$	$\theta [\text{deg}], ^3J_{\text{HH}} [\text{Hz}]$ eq. 17	$\theta_{\text{X}}^{\text{A}} [\text{deg}]$	$\theta [\text{deg}], ^3J_{\text{HH}} [\text{Hz}]$ eq. 19, 20
1	4.1		0.3439	20.11, 4.18	2.907	21.93 <sup>U1C1</sup> , 4.12	33.82	22.35 <sup>U2B1</sup> , 4.11
		3.08						
2	5.4	4.49	0.0203	-28.83, 5.45	49.09	-24.54 <sup>U1E1</sup> , 5.35	-	-
		4.38						
3	0 d, H <sub>3</sub> , 0.1	3.22	0.0862	-94.96 <sup>S1B4</sup> , 1.1 <sup>tan</sup> -92.47 <sup>S1E4</sup> , 0.79 <sup>tan</sup>	0.203 0.086 0.862	-24.96 <sup>U1G1</sup> , 5.36 -90.08 <sup>S1B4</sup> , 0.146 <sup>tan</sup> -90.86 <sup>S1B4</sup> , 0.46 <sup>tan</sup>	0.165 0.029 2.972	-24.97 <sup>U1G1</sup> , 5.36 -90.029 <sup>S1B4</sup> , 0.086 <sup>tan</sup> -92.97 <sup>S1B4</sup> , 0.86 <sup>tan</sup>
4	3.1		0.1451	51.65 <sup>U1A2</sup> , 3.09	6.888	51.88 <sup>U2F2</sup> , 3.08 50.24 <sup>U1D2</sup> , 3.15	189.82 8.428	50.172 <sup>U1A2</sup> , 3.15 51.571 <sup>U1A2</sup> , 3.09
		3.71						
5	3.9	4.16	0.0256	29.26 <sup>S1E1</sup> , 3.89	39.00	25.2 <sup>S1G1</sup> , 4.01 29.74 <sup>S1B1</sup> , 3.88	-	-
		4.26						
6	8.8	3.58	0.0772	-166.88 <sup>U1F6</sup> , 8.78 <sup>tan</sup>	12.941	-166.71 <sup>U1A6</sup> , 8.77 <sup>tan</sup> -169.57 <sup>U1B6</sup> , 8.92 <sup>tan</sup>	167.47 0.597	-167.16 <sup>U1A6</sup> , 8.8 <sup>tan</sup> -169.63 <sup>U1B6</sup> , 8.93 <sup>tan</sup>
7	4.8		0.1895	-2.78 <sup>S1A1</sup> , 4.81	5.274	-1.64 <sup>U1S1A1</sup> , 4.78 -1.89 <sup>S1A1</sup> , 4.79	111.290 14.376	-3.87 <sup>U1S1A1</sup> , 4.84 -1.86 <sup>S1B1</sup> , 4.79
		3.11						
8	5.2	4.02	0.0192	-15.55 <sup>U1G1</sup> , 5.13 -19.66 <sup>U1A1</sup> , 5.23	51.999	-19.00 <sup>U1G1</sup> , 5.22 -19.93 <sup>U1A1</sup> , 5.24	-	-
		4.12						
9	0 bs, 0.81	2.89	0.6585	-93.57 <sup>S1A4</sup> , 0.94 <sup>tan</sup>	0.658	-90.65 <sup>S1B4</sup> , 0.4 <sup>tan</sup> -93.29 <sup>SD1</sup> , 0.90 <sup>tan</sup>	1.7346 173.46	-91.73 <sup>S1B4</sup> , 0.65 <sup>tan</sup> -93.27 <sup>SE4</sup> , 0.90 <sup>tan</sup>

[a]  $\delta[\text{ppm}]$  1-CDCl<sub>3</sub>, 2-D<sub>2</sub>O, 3- CDCl<sub>3</sub>: <sup>13</sup>C 75 [MHz], <sup>1</sup>H 400 [MHz]

3-Sphere approach for calculation of the dihedral angles from NMR data, under Hopf fibration and Lie algebra, follow few steps:

1. Calculation of the dihedral angles only from vicinal coupling constant with Java Script program PRE-DICTIEACS2022.html. [7] The program of prediction is based on trigonometric equation and not on algebraic equations. The differences between *trans-ee*<sup>4,1</sup> and *trans-ee*<sup>3,2</sup> ( $\theta^3$  and  $\theta^4$ ) can be made only with algebraic equations on very good recorded spectra, probably. The transformation from U to S is performed with *trans-ee*<sup>3,2</sup> algebraic equation, almost compatible with *tan* function, a general rule for calculation only the *trans-ee*<sup>3,2</sup> angle, [11] but from trigonometric equations, and algebraic equation for *trans-ee*<sup>4,1</sup>, first angle of set A or B, is too hard to made the differences between the two *trans-ee* angles. From eq. 25, 26 results *cis*- $\theta^{\text{SA1}}$

angles with negative sign giving *trans-ee*<sup>4,1</sup> dihedral angles in accord with D-ribitol stereochemistry.

2. Calculation one angle of set A with manifold equations from carbon and/or proton chemical shift.
3. Building of seven sets angles of unit U and S, and choosing the dihedral angle with values almost equals with calculated dihedral angles from vicinal coupling constant. The number of unit U and S can be increased through set C until the angles of first unit are almost equals with last unit, at list can be extracted and analyzed the differences results from chemical shift for many dihedral angles with values almost equals with dihedral angles calculated only from vicinal coupling constant.
4. Calculation of the vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  of the manifold dihedral angles.

**Table 2.** Dihedral angles of iminocyclitols 1-3 calculated from differences between chemical shift of two carbon  $\Delta\delta_{Cn}[\text{ppm}]$  and vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$  with polar equations 18, 19, 20.

Entry	$^3J_{\text{HH}}^{\text{a}}$ [Hz]	$C_n$ [ppm]	$R_{\text{mC}}$ [°]	$\theta[\text{deg}], ^3J_{\text{HH}}[\text{Hz}]$	$\theta^{\text{A}}$ [deg]	$\theta[\text{deg}], ^3J_{\text{HH}}[\text{Hz}]$ eq. 18	$\theta_{\text{X}}^{\text{A}}$ [deg]	$\theta[\text{deg}], ^3J_{\text{HH}}[\text{Hz}]$ eq. 19, 20
1	4.1	55.8	0.1480	$21.48^{\text{U1B1}}, 4.13$	6.756	$23.48^{\text{U1B1}}, 4.13$	182.57	$21.71^{\text{U1C1}}, 4.13$
		83.5			1.480	$20.98^{\text{U1C1}}, 4.15$	8.763	$21.23^{\text{U1B1}}, 4.14$
2	5.4	84.3	0.1481	$-25.74^{\text{S1E1}}, 5.37$	6.75	$-26.62^{\text{S1E1}}, 5.39$	182.25	$-27.75^{\text{S1B1}}, 5.42$
		65.9			1.481	$-28.51^{\text{S1B1}}, 5.44$	8.779	$-25.61^{\text{S1E1}}, 5.37$
3	0 d, H <sub>3</sub>		0.0054	$-90.308^{\text{S1B4}}, 0.277^{\text{tan}}$	0.0054	$-90.005^{\text{S1B4}}, 0.036^{\text{tan}}$	0.0001	$-90.0001^{\text{S1B4}}, 0.005^{\text{tan}}$
					0.0543	$-90.053^{\text{S1B4}}, 0.115^{\text{tan}}$	0.0118	$-90.0118^{\text{S1B4}}, 0.053^{\text{tan}}$
4	3.1	57.4	0.2198	$51.35^{\text{U1F2}}, 3.108$ $(-31.98, -53.10^{\text{tan}})$	4.548	$50.90^{\text{U1C2}}, 3.12$	82.751	$52.75^{\text{U1B2}}, 3.05$
		71.5			2.198	$49.26^{\text{U1B2}}, 3.19$	19.335	$50.33^{\text{U1D2}}, 3.14$
5	3.9	71.7	0.0512	$28.53^{\text{S1E1}}, 3.92$	19.499	$28.49^{\text{S1A1}}, 3.92$	-	-
		66.8			0.512	$29.48^{\text{S1B1}}, 3.88$	1.0519	$28.94^{\text{S1B1}}, 3.90$
6	8.8		0.5568	$-168.49^{\text{U1F6}}, 8.87^{\text{tan}}$	1.7959	$-169.21^{\text{U1F6}}, 8.91^{\text{tan}}$	3.225	$-168.71^{\text{U1F6}}, 8.88^{\text{tan}}$
					5.5681	$-167.49^{\text{U1F6}}, 8.81^{\text{tan}}$	31.004	$-169.49^{\text{U1F6}}, 8.92^{\text{tan}}$
7	4.8	63.7	0.5454	$-3.055^{\text{S1B1}}, 4.82$ $(-44.95, 3.06^{\text{tan}})$	1.8333	$-1.833^{\text{S1A1}}, 4.79$	13.444	-
		72.5			5.4545	$(-44.98, 3.06^{\text{tan}})$	119.008	$-1.983^{\text{S1C1}}, 4.79$
8	5.2	74.0	0.2884	$-16.76^{\text{U1A1}}, 5.16$ $(-43.75, 17.53^{\text{tan}})$	3.4666	$(-44.96, 2.73^{\text{tan}})$		$(-44.98, 1.98^{\text{tan}})$
		69.3			2.8846	$-18.84^{\text{U1A1}}, 5.21$		$-18.07^{\text{U1B1}}, 5.19$
9	0 bs, 0.81		0.1723	$-90.182^{\text{S1B4}}, 0.213^{\text{tan}}$	5.8024	$(-43.42, 19.95^{\text{tan}})$	48.0711	$(-43.55, 19.04^{\text{tan}})$
					1.7234	$-19.03^{\text{U1A1}}, 5.22$	33.2840	$-18.90^{\text{U1A1}}, 5.21$
						$(-43.38, 20.18^{\text{tan}})$		$(-43.41, 20.02^{\text{tan}})$
						$-95.772^{\text{S1B4}}, 1.20^{\text{tan}}$	134.674	$-91.953^{\text{S1CB4}}, 0.698^{\text{tan}}$
						$-91.724^{\text{S1B4}}, 0.656^{\text{tan}}$	11.8804	$-95.668^{\text{S1CB4}}, 1.187^{\text{tan}}$

[a]  $\delta[\text{ppm}]$  1-CDCl<sub>3</sub>, 2-D<sub>2</sub>O, 3- CDCl<sub>3</sub>; <sup>13</sup>C 75 [MHz], <sup>1</sup>H 400 [MHz].

## 4. Conclusions

3-Sphere approach, a method which enables calculation of the dihedral angles, tetrahedral angles, bond lengths, from chemical shift  $\delta[\text{ppm}]$  and vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$ , was analyzed in this paper from the manifold point of view in attempt to find the best solution for building a program for calculation of the conformation and configuration of five and six membered ring, based on spatial representation.

Five Java Script programs for calculation dihedral angles from NMR data, carbon and/or proton chemical shift  $\delta[\text{ppm}]$  along vicinal coupling constant  $^3J_{\text{HnHn+1}}[\text{Hz}]$ , with manifold equations of 3-Sphere approach are presented in Fig. 1, 3-6: rectangle, Villarceau circles of cyclide (Torus – Dupin Cyclide), polar equations, Euler-Conic, and unit of seven sets angles.

## Abbreviations

RMN Nuclear Magnetic Resonance

## Author Contributions

**Carmen-Irena Mitani:** Conceptualization, Methodology, Writing – original draft, Writing – review & editing  
**Emerich Bartha:** Conceptualization, Metodology  
**Petru Filip:** Methodology  
**Miron-Teodor Caproiu:** Formal Analysis  
**Constantin Draghici:** Methodology  
**Robert Michael Moriarty:** Supervision

## Conflicts of Interest

The authors declare no conflicts of interest.



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