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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 δ_{Xn}[ppm] and vicinal coupling constant $^{3}J_{HnHn+1}$[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.* lima ons or cardioid, rose or lemniscale), 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, Reactangle, 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 (Kahler structure), algebraic (sphere, Riemannian sphere, torus – elliptic curves – Weierstrass elliptic functions). [2] Sixteen points on the Poincar ésphere results from four points of polar angle and azimuthal angle in case of Poincar érotator, a polarization modulator, which enable dynamic control over a polarization state by execution an arbitrary rotation on the Poincar é sphere, same with Poincar é sphere on organic stereochemistry. The Poincar é rotor is an SU(2) Lie group operator, with two U(1) operations to change the phase and the

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amplitude of the state, able to achieve distinguishable 4x4 = 16, 8x8 = 64, 10x10 = 100 states on the Poincaré sphere after modulating both the phase and amplitude. The molecular structure of Buckmmsterfullerene (C60) 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. Minlowski 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_o with unique four dimension manifold M, in fact the Euclidean space E^3 of M_o is replaced by a sphere S^3 of small but nonvanishing curvature, a deformation of M into M_o, 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 algebara. [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 cons having six dihedral angle and two algebraic angles, $3x\phi_1$ and $2x\phi_2$, which after translation from 3D to 2D can be represented on two sets angles having as point of linkage halt of ϕ_1 of sets A and B equal with first angle of set B and A. First angles of sets A and B are equals ϕ_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 φ_{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 φ_{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 transformed 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 θ and ϕ.

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^{6,1}

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^{6,1}

where: θ^{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>
<title1>A Java script including HTML</title1>

</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><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><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><i>J</i><sub>HH</sub>[Hz]</b>=",usedataZ);
document.write("<p><i>Trans-aa</i> HnHn+1:",usedataZZ);

var usedata1A
usedata1A = prompt ("Value of Cn[ppm]")

var usedata1B
usedata1B = prompt ("Value of Cm[ppm]")

//calculate the difference in chemical shifts between two atoms of carbon
var CnCm = usedata1A - usedata1B;//CnCm in ppm

if (CnCm < 0){
var CnCm = usedata1B - usedata1A;//CnCm in ppm
}
else {
var CnCm = usedata1A - usedata1B;//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 = ",usedata1A);
document.write("<p>Cm[ppm] type in = ",usedata1B);
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 IHnHm[ppm] the inverse of HnHm[ppm]
var IHnHm = 1/HnHm;//IHnHm in 1/ppm

if (HnHm < 1){
var IHnHm = 1/HnHm;//IHnHm in 1/ppm
}
else{
var IHnHm = HnHm;//IHnHm 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> (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> (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> (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>");
document.write("<p><B>Case IIa</B> (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> (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 IIc</B> (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 IId</B> (C + 1/H, m = 1): 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> (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 IIIb</B> (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> (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> (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> (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> (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> (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><i>J</i><sub>HnHm</sub> higher as 9.5[Hz].</h4>");
 document.write("<p><B>Case VI</B> (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 δ[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 $^3J_{HnHn+1}$[Hz] from vicinal angle ϕ[deg] (eq. 5-8).

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

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

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

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

Java Script program presented at ACS spring 2021 for calculation of the dihedral angles from carbon and proton chemical shift δ_{Cn}[ppm] with rectangle equations in 3 steps [13]: 1. Prediction of de dihedral angles θ_{HnHn+1}[deg] only from vicinal coupling constants ${}^{3}J_{HnHn+1}$[Hz] without torus inversion; 2. Calculation the first angle of set B or half ϕ_1 of set A; 3. Building three sets angles for all equations (eq. 1-4), 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]

2.1.2. Cyclide Approach

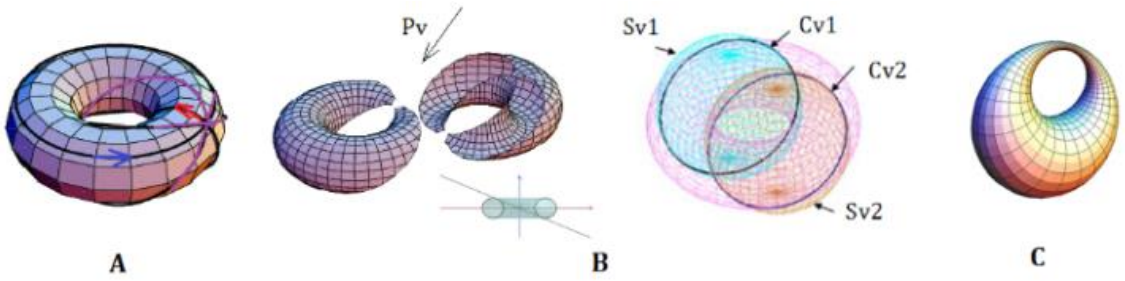

Figure 2. *Torus (A) and Dumpin Cyclide (C).*

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]

$$\theta_T^{NA} = \sin^{-1}\left(\frac{\Delta\delta HH}{\Delta\delta CC}\right) \quad (9)$$

$$\theta_T^{NB} = \cos^{-1}\left(\frac{\Delta\delta HH}{\Delta\delta CC}\right) \quad (10)$$

$$\theta_D^{NA} = \tan^{-1}\left(\frac{\Delta\delta HH}{\Delta\delta CC}\right) \quad (11)$$

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

Where: $\Delta\delta_{HnHn+1}$, $\Delta\delta_{CnCn+1}$ – the differences between two consecutive protons and two atoms of carbon [ppm], $\theta_T^{NA, NB}$, $\theta_D^{NA, NB}$ - 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 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]:

$$\theta_W^{nA} = \sin^{-1}(\Delta\delta_{HnHn+1} x \omega_H / \Delta\delta_{CnCn+1} x \omega_C) \quad (13)$$

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

B. *Transformation in gauss:*

$$\theta_W^{nA} = \sin^{-1}(\Delta\delta_{HnHn+1} x \omega_H/\gamma_H / \Delta\delta_{CnCn+1} x \omega_C/\gamma_C) \quad (15)$$

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

Where: $\Delta\delta_{HnHn+1}$, $\Delta\delta_{CnCn+1}$ – the differences between two consecutive protons and two atoms of carbon [ppm], ω_L – Larmor frequency [^{13}C: 75MHz, ^{1}H 400MHz], ν – frequency [Hz], δ – chemical shifts [ppm], γ – gyromagnetic ratio: ^{13}C: γ = 10.71 [MHzxT^{-1}] = 6.7[10^{7}xradxT^{-1}xs^{-1}], ^{1}H: γ = 42.57 [MHzxT^{-1}] = 26.7[10^{7}xradxT^{-1}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><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><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><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 δ[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><i>J</i><sub>HH</sub>[Hz]</b>=",usedata1)
document.write("<p><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><i>J</i><sub>HH</sub>[Hz]</b>=",usedata2)
 document.write("<p><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 Xm[ppm] =",usedata4);
 document.write("<p>The value of XnXm[ppm] ="+XnXm);

var usedata5
usedata5 = XnXm/usedata1;//calculate the value of RcJc
var RcJc = usedata5;//value of RcJc

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

 var RcJc = 1/usedata5;//value of RcJc
      }

 var Rc = Math.asin(RcJc);//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 CJc = RcJc;// value of CJc

      if (RcJc < 1){
      //calculate angle CJc in deg for cis stereochemistry
      var CJc = 1/RcJc;//angle CJc[deg]
      }
      else{
      var CJc = RcJc;//angle CJc[deg]
      }

 var DJc = 10*RcJc;// value of DJc

 var AJcs = (2*CJc);// value of AJcs
 var AJcf = AJcs*AJcs;// value of AJcf[deg]

 var BJcs = (2*DJc);// value of BJcs
 var BJcf = (BJcs*BJcs);// value of BJcf[deg]

 //calculate angles with trans-ee stereochemistry
 var CJe = RcJc;// value of CJe

      if (RcJc > 1){
      //calculate angle CJe in deg for trans-ee stereochemistry
      var CJe = 1/RcJc;//angle CJe[deg]
      }
      else{
      var CJe = RcJc;//angle CJc[deg]
      }

  var DJe = 10*RcJc;// value of DJe

  var AJes = (2*CJe);// value of AJes
  var AJef = AJes*AJes;// value of AJef[deg]

  var BJes = (2*DJe);// value of BJes
  var BJef = (BJes*BJes);// value of BJef[deg]

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

  document.write("<p><i>A. Transformation under stereochemistry and unit
  rule</i>.</p>");
  document.write("<p><i>cis</i>: AJcf[deg] ="+AJcf);

document.write("<p><i>cis</i>: BJcf[deg] ="+BJcf);
document.write("<p><i>trans-ee</i>: AJef[deg] ="+AJef);
document.write("<p><i>trans-ee</i>: BJef[deg] ="+BJef);

document.write("<p><i>B. Transformation under unit rule</i>.</p>");
document.write("<p><i> RcJc[deg] ="+RcJc);
document.write("<p><i> Rcd[deg] ="+Rcd);
document.write("<p><i>cis</i>: CJc[deg] ="+CJc);
document.write("<p><i>cis</i>: DJc[deg] ="+DJc);
document.write("<p><i>trans-ee</i>: CJe[deg] ="+CJe);
document.write("<p><i>trans-ee</i>: DJe[deg] ="+DJe);

var usedata6
usedata6 = XnXm/usedata2;//calculate the value of RtJt
var RtJt = usedata6;//value of RtJt for trans-aa stereochemistry

//calculate the angle of set A[deg] for trans-aa stereochemistry
var Rt = Math.asin(RtJt);//the dihedral angle Rt[rad] with trans stereochemistry
var Rtd = (Rt)*(57.29577521);//the dihedral angle Rtd[deg] with trans
stereochemistry

//calculate the angle of set A[deg] for trans-aa stereochemistry
var CJt = RtJt;// value of CJt

if (RtJt < 1){
      //calculate angle CJt in deg
      var CJt = 1/RtJt;//angle CJt[deg]
      }
      else{
      var CJt = RtJt;//angle CJt[deg]
      }

var DJt = 10*RtJt;//value of DJt[deg]

var AJtf = CJt*CJt;// value of AJtf[deg]
var BJtf = (DJt*DJt);// value of BJtf[deg]

document.write("<p><b>II.Trans-aa stereochemistry</b>.</p>");
document.write("<p><i>A.Transformation under stereochemistry and unit
rule</i>.</p>");
document.write("<p><i>trans-aa</i>: AJtf[deg] ="+AJtf);
document.write("<p><i>trans-aa</i>: BJtf[deg] ="+BJtf);
document.write("<p><i>B.Transformation under unit rule</i>.</p>");
document.write("<p><i>trans-aa</i>: RtJt[deg] ="+RtJt);
document.write("<p><i>trans-aa</i>: Rtd[deg] ="+Rtd);
document.write("<p><i>trans-aa</i>: CJt[deg] ="+CJt);
document.write("<p><i>trans-aa</i>: DJt[deg] ="+DJt);

alert("Hello World!");

</script>
</body>
</html>
```

Figure 4. *Java Script program SciencePOLAReq.html for calculation of dihedral angles with polar equations 17-20 from carbon chemical shift δ[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 π to deg) are proposed for calculation of dihedral angles θ_{HnHn+1}[deg] from the ratio differences in chemical shift between two protons or atoms of carbon and vicinal coupling constant $^3J_{HnHn+1}$[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 $\Delta\nu = J\text{x}(3)^{1/2}$ at smaller differences of two protons chemical shift, in other words from AB to AX coupling. [17]

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

$$R_{mC} = \Delta\delta_{CnCn+1}/^3J_{HnHn+1}[s] \quad (18)$$

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

$$\textit{cis, trans-ee}: (2\text{x}R_{mH})^2 = \theta_x \quad (19)$$

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

$$(\nu_4 - \nu_1)/(\nu_3 - \nu_2) = \tan^2\theta \quad (21)$$

$$(\nu_1 - \nu_3) = (\nu_2 - \nu_4) = (\Delta\nu^2 + J^2)^{1/2} \quad (22)$$

Where ν_n – n = 1 – 4, four pics of the two coupled protons.

```
<!DOCTYPE html>
<html>
<head>
<title1>A Java script including HTML</title1>

</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 usedata1a
usedata1a = prompt ("Value of Hn[ppm]")
var usedata1b
usedata1b = prompt ("Value of Hm[ppm]")

//calculate the value of CnCm[ppm]

var HnHm = usedata1a - usedata1b;//the differences between two
protons in ppm

if (HnHm < 0){
var HnHm = usedata1b - usedata1a;//the differences between two
protons in ppm
}
else{
var HnHm = usedata1a - usedata1b;//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>The Hn[ppm] type in=",usedata1a);
document.write("<p>The Hm[ppm] type in=",usedata1b);
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="+Ah1);
document.write("<p>The angle U1Bh1[deg] is="+Bh1);

var usedata3a
usedata3a = prompt ("Value of Cn[ppm]")
var usedata3b
usedata3b = prompt ("Value of Cm[ppm]")

//calculate the value of CnCm[ppm]
var CnCm = usedata3a - usedata3b

if (CnCm < 0){
var CnCm = usedata3b - usedata3a;
}
else{
var CnCm = usedata3a - usedata3b;
}

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 $R_{mx} = \Delta\delta_{XnXn+1}x\omega_H x4x10^{-3}/\gamma_H$ [gauss], x = C, H; $\Delta\delta_{XnXn+1}$ – the differences between two consecutive protons and two atoms of carbon [ppm], ω_L – Larmor frequency [^{13}C: 75MHz, ^{1}H 400MHz], ν – frequency [Hz], δ – chemical shifts [ppm], γ – gyromagnetic ratio.

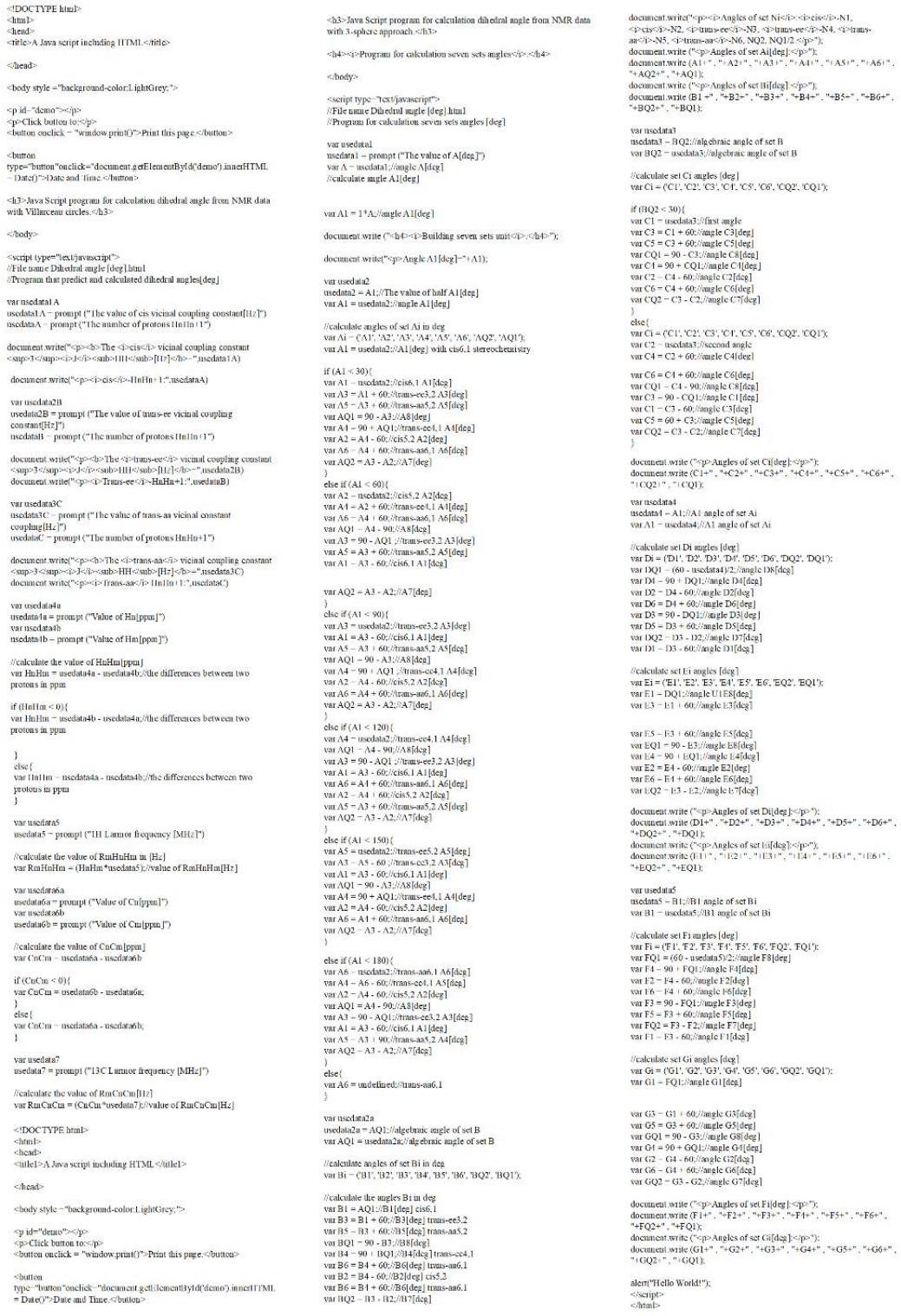

Figure 6. *Java Script program ScienceSevenUnit.html for building seven sets units.*

Java Script program EulerConic.html for calculation of the dihedral angles from carbon or proton chemical shift with Euler-Conic eq. 23 is presented in Figure 5. Same with all the programs presented in this paper, is a short program only for calculation one angle of first set. With the angle calculated then can be used a program for building of the units with seven sets angles from sin or tan function, and used the transformation from U to S and S to U published already [11]. A program for calculation of two seven sets units starting with half ϕ_1 of set A namely AQ1 was presented at ASC spring 2021 (Step3unitAQ1.html). As reported by Silverstein, G. C. Bassler difference between chemical shift of two coupled

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 θ^{UB1} leading to third angles of set θ^{SA3} with eq. 24.

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

Where: θ^{UB1} – first angle of set B from unit U ($\theta^{N1} > 5$[deg]), θ^{SB3} – third angle of set B from unit S ($\theta^{N1} < 5$[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[deg], S1A1 < 5[deg], i = 1-6.

3. Discussion

The Java Script programs presented for calculation from chemical shift δ[ppm] and/or vicinal coupling constant $^3J_{HnHn+1}$[Hz] enable a carefully analysis of dihedral angles θ_{HnHn+1}[deg] with corresponding sign and stereochemistry. Since bond distances l_{CnCn+1}[A^0] between two atoms of carbon are all under different polar equations (*i.e.* limaçons or cardioid, rose or lemniscale) 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 θ_{HnHn+1}[deg] and tetrahedral angles φ_{Cn}[deg] in opposite. [8]

Villarceau approach (eq. 9-12) and Java Script program ScienceVillarceau.html (Figure 3) enable calculation of the dihedral angles θ_{HnHn+1}[deg] from the ratio proton/carbon chemicals shift δ[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 s*in* function.

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

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

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 $\Delta\delta_{HnHn+1}$[ppm] or two carbons chemical shift $\Delta\delta_{CnCn+1}$[ppm] and vicinal coupling constant $^3J_{HnHn+1}$[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 (θ^A, $\theta_X{}^A$[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 θ_{HnHn+1}[deg] calculated only from vicinal coupling constant $^3J_{HnHn+1}$[Hz]In accord with D-ribitol stereochemistry, iminocyclitols 1-3 [18] (Figure 7) have negative dihedral angle θ_{H3H4}[deg], angle calculated with equations 25, 26.

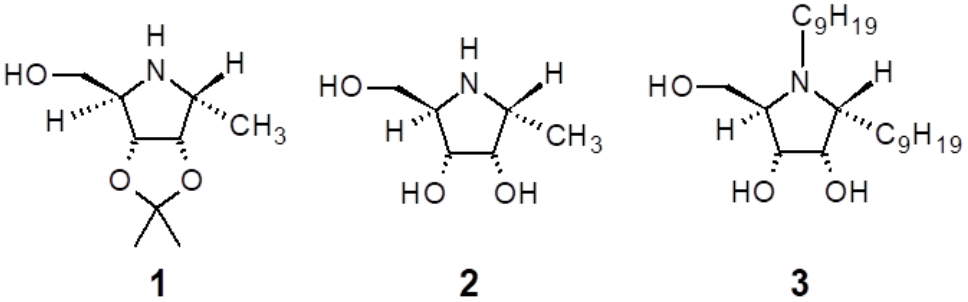

Figure 7. *Iminocyclitols 1-3 with C_1-R-α-Dribitol stereochemistry [18].*

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

Entry	$^{3}J_{HH}$[a] [Hz]	H_n [ppm]	R_{mH} [π]	θ[deg], $^{3}J_{HH}$[Hz]	θ^{A} [deg]	θ[deg], $^{3}J_{HH}$[Hz] eq. 17	θ_X^{A} [deg]	θ[deg], $^{3}J_{HH}$[Hz] eq. 19, 20
1	4.1	3.08	0.3439	20.11, 4.18	2.907 3.439	21.93^{U1C1}, 4.12 22.29^{U1C1}, 4.11	33.82 47.30	22.35^{U2B1}, 4.11 23.65^{U1E1}, 4.07
2	5.4	4.49	0.0203	-28.83, 5.45	49.09	-24.54^{U1E1}, 5.35	-	-
3	0 d, H_3, 0.1	4.38 3.22	0.0862	-94.96^{S1B4}, 1.1^{tan} -92.47^{S1E4}, 0.79^{tan}	0.203 0.086 0.862	-24.96^{U1G1}, 5.36 -90.08^{S1B4}, 0.146^{tan} -90.86^{S1B4}, 0.46^{tan}	0.165 0.029 2.972	-24.97^{U1G1}, 5.36 -90.029^{S1B4}, 0.086^{tan} -92.97^{S1B4}, 0.86^{tan}
4	3.1	3.71	0.1451	51.65^{U1A2}, 3.09	6.888 1.451	51.88^{U2F2}, 3.08 50.24^{U1D2}, 3.15	189.82 8.428	50.172^{U1A2}, 3.15 51.571^{U1A2}, 3.09
5	3.9	4.16 4.26	0.0256	29.26^{S1E1}, 3.89	39.00 0.256	25.2^{S1G1}, 4.01 29.74^{S1B1}, 3.88	- 0.262	- 29.73^{S1B1}, 3.88
6	8.8	3.58	0.0772	-166.88^{U1F6}, 8.78^{tan}	12.941 0.772	-166.71^{U1A6}, 8.77^{tan} -169.57^{U1B6}, 8.92^{tan}	167.47 0.597	-167.16^{U1A6}, 8.8^{tan} -169.63^{U1B6}, 8.93^{tan}
7	4.8	3.11	0.1895	-2.78^{S1A1}, 4.81	5.274 1.895	-1.64^{U1S1A1}, 4.78 -1.89^{S1A1}, 4.79	111.290 14.376	-3.87^{U1S1A1}, 4.84 -1.86^{S1B1}, 4.79
8	5.2	4.02 4.12	0.0192	-15.55^{U1G1}, 5.13 -19.66^{U1A1}, 5.23	51.999 0.192	-19.00^{U1G1}, 5.22 -19.93^{U1A1}, 5.24	- 0.1479	- -19.95^{U1A1}, 5.24
9	0 bs, 0.81	2.89	0.6585	-93.57^{S1A4}, 0.94^{tan}	0.658 6.585	-90.65^{S1B4}, 0.4^{tan} -93.29^{SD1}, 0.90^{tan}	1.7346 173.46	-91.73^{S1B4}, 0.65^{tan} -93.27^{SE4}, 0.90^{tan}

[a] δ[ppm] 1-$CDCl_3$, 2-D_20, 3- $CDCl_3$: ^{13}C 75 [MHz], ^{1}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 PREDICTIEACS2022.html. [7] The program of prediction is based on trigonometric equation and not on algebraic equations. The differences between *trans-ee*^{4,1} and *trans-ee*^{3,2} (θ^3 and θ^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*^{3,2} algebraic equation, almost compatible with *tan* function, a general rule for calculation only the *trans-ee*^{3,2} angle, [11] but from trigonometric equations, and algebraic equation for *trans-ee*^{4,1}, 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*-θ^{SA1} angles with negative sign giving *trans-ee*^{4,1} 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 $^{3}J_{HnHn+1}$[Hz] of the manifold dihedral angles.

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

Entry	$^3J_{HH}$ [a] [Hz]	C_n [ppm]	R_{mC} [π]	θ[deg], $^3J_{HH}$[Hz]	θ^A [deg]	θ[deg], $^3J_{HH}$[Hz] eq. 18	θ_X^A [deg]	θ[deg], $^3J_{HH}$[Hz] eq. 19, 20
1	4.1	55.8	0.1480	21.48^{U1B1}, 4.13	6.756 1.480	23.48^{U1B1}, 4.13 20.98^{U1C1}, 4.15	182.57 8.763	21.71^{U1C1}, 4.13 21.23^{U1B1}, 4.14
2	5.4	83.5 84.3	0.1481	-25.74^{S1E1}, 5.37	6.75 1.481	-26.62^{S1E1}, 5.39 -28.51^{S1B1}, 5.44	182.25 8.779	-27.75^{S1B1}, 5.42 -25.61^{S1E1}, 5.37
3	0 d, H_3	65.9	0.0054	-90.308^{S1B4}, 0.277 ^{tan}	0.0054 0.0543	-90.005^{S1B4}, 0.036 ^{tan} -90.053^{S1B4}, 0.115 ^{tan}	0.0001 0.0118	-90.0001^{S1B4}, 0.005 ^{tan} -90.0118^{S1B4}, 0.053 ^{tan}
4	3.1	57.4	0.2198	51.35^{U1F2}, 3.108 (-31.98, -53.10^{tan})	4.548 2.198	50.90^{U1C2}, 3.12 49.26^{U1B2}, 3.19	82.751 19.335	52.75^{U1B2}, 3.05 50.33^{U1D2}, 3.14
5	3.9	71.5 71.7	0.0512	28.53^{S1E1}, 3.92	19.499 0.512	28.49^{S1A1}, 3.92 29.48^{S1B1}, 3.88	- 1.0519	- 28.94^{S1B1}, 3.90
6	8.8	66.8	0.5568	$-168.49^{U1\mathbf{F6}}$, 8.87^{tan}	1.7959 5.5681	$-169.21^{U1\mathbf{F6}}$, 8.91^{tan} $-167.49^{U1\mathbf{F6}}$, 8.81^{tan}	3.225 31.004	$-168.71^{U1\mathbf{F6}}$, 8.88^{tan} $-169.49^{U1\mathbf{F6}}$, 8.92^{tan}
7	4.8	63.7	0.5454	-3.055^{S1B1}, 4.82 (-44.95, 3.06^{tan})	1.8333 5.4545	-1.833^{S1A1}, 4.79 (-44.98, 3.06^{tan}) -2.727^{S1D1}, 4.81 (-44.96, 2.73^{tan})	13.444 119.008	- -1.983^{S1C1}, 4.79 (-44.98, 1.98^{tan})
8	5.2	72.5 74.0 69.3	0.2884	-16.76^{U1A1}, 5.16 (-43.75, 17.53^{tan})	3.4666 2.8846	-18.84^{U1A1}, 5.21 (-43.42, 19.95^{tan}) -19.03^{U1A1}, 5.22 (-43.38, 20.18^{tan})	48.0711 33.2840	-18.07^{U1B1}, 5.19 (-43.55, 19.04^{tan}) -18.90^{U1A1}, 5.21 (-43.41, 20.02^{tan})
9	0 bs, 0.81		0.1723	-90.182^{S1B4}, 0.213 ^{tan}	5.8024 1.7234	-95.772^{S1B4}, 1.20 ^{tan} -91.724^{S1B4}, 0.656 ^{tan}	134.674 11.8804	-91.953^{S1CB4}, 0.698 ^{tan} -95.668^{S1CB4}, 1.187 ^{tan}

[a] δ[ppm] 1-$CDCl_3$, 2-D_20, 3- $CDCl_3$: ^{13}C 75 [MHz], ^1H 400 [MHz].

4. Conclusions

3-Sphere approach, a method which enables calculation of the dihedral angles, tetrahedral angles, bond lengths, from chemical shift δ[ppm] and vicinal coupling constant $^3J_{HnHn+1}$[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 δ[ppm] along vicinal coupling constant $^3J_{HnHn+1}$[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 Mitan: Conceptualization, Methodology, Writing – original draft, Writing – review & editing
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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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