Two Mathematical Proofs of Bond Angle in a Regular Tetrahedral Structure

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1. Introduction: This paper presents a proof of the angle between any two bonds in a molecule possessing a tetrahedral structure, such as the methane molecule, in which all four σ-bonds (corresponding to four hydrogen atoms bonded to a central carbon atom) are equally inclined in three-dimensional space. The bond angle is derived using two independent approaches. The first method involves formulating the geometry of a right pyramid with a regular n-gonal base [1], while the second employs HCR's formula for regular polyhedral [2]. Both approaches lead to the same result, thereby providing a simple and rigorous geometric justification of the tetrahedral bond angle.

2. Method-1: Using the equation of right pyramid with regular n-polygonal base

2.1. Relation between angles α & β in a right pyramid with base as a regular n-polygon

Let there be a right pyramid with base as a regular polygon $A_1A_2A_3 \dots . A_n$ having 'n' no. of sides each of length 'a', angle between any two consecutive lateral edges $'\alpha'$, normal height 'H' & an acute angle $'\beta'$ of the axis PO with any of the lateral edges (as shown in the figure 1).

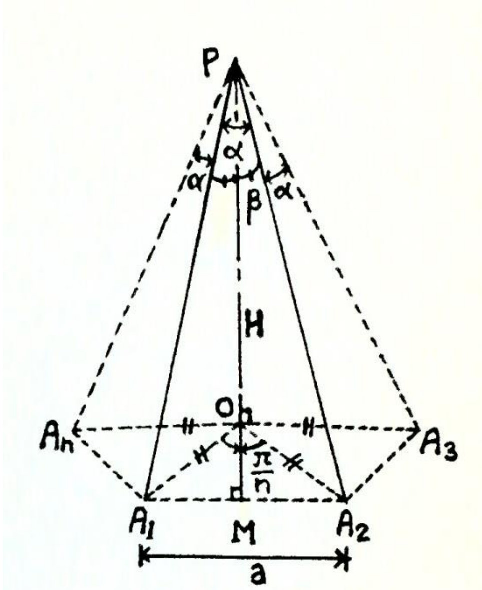

Figure 1: A right pyramid having base as a regular polygon with each side a, angle between any two consecutive lateral edges $= \alpha$ & angle of the geometrical axis PO with each of the lateral edges $= \beta$.

Now, join all the vertices $A_1, A_2, A_3, \dots . A_n$ of the base to the centre 'O' thus we obtain 'n' no. of congruent isosceles triangles $\Delta A_1OA_2, \Delta A_2OA_3 \dots \dots \dots . \Delta A_nOA_1$

In right ΔOMA_2 (Fig. 1),

$$\Rightarrow \tan \angle A_2OM = \frac{MA_2}{OM}$$

$$or \ \ tan\frac{\pi}{n} = \frac{\left(\frac{a}{2}\right)}{OM} \qquad \Rightarrow \ OM = \frac{a}{2}cot\frac{\pi}{n} \quad \left(\because \angle A_2OM = \frac{\pi}{n}\right)$$

In right ΔPOM (Fig. 1),

$$\Rightarrow \ PM^2 = OP^2 + OM^2 \ \ or \ PM = \sqrt{H^2 + \left(\frac{a}{2}cot\frac{\pi}{n}\right)^2}$$

$$\Rightarrow \ \boldsymbol{PM = \frac{1}{2}\sqrt{4H^2 + a^2cot^2\frac{\pi}{n}}} \qquad \dots \dots \dots \dots \dots (I)$$

In right ΔPMA_2 (Fig. 1),

$$\Rightarrow \tan \angle A_2PM = \frac{MA_2}{PM}$$

$$\Rightarrow \ tan\frac{\alpha}{2} = \frac{\left(\frac{a}{2}\right)}{PM} \ \ or \ \ \boldsymbol{PM = \frac{a}{2}cot\frac{\alpha}{2}} \qquad \dots \dots \dots \dots \dots . (II)$$

Now, equating the values of **PM** from equation (I) & (II), we have

$$\Rightarrow \frac{a}{2}cot\frac{\alpha}{2} = \frac{1}{2}\sqrt{4H^2 + a^2cot^2\frac{\pi}{n}}$$

On squaring both the sides, we get

$$a^2cot^2\frac{\alpha}{2} = 4H^2 + a^2cot^2\frac{\pi}{n} \qquad \Rightarrow 4H^2 = a^2\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)$$

$$\boldsymbol{H = \frac{a}{2}\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}}} \quad \forall\ \boldsymbol{n \geq 3} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots.(III)$$

Above is the generalised formula for calculating the normal height H of any right pyramid having base as a regular polygon with n no. of sides each of length a & an angle α between any two consecutive lateral edges [1].

Now, in right ΔOMA_2 (Fig. 1),

$$\Rightarrow \sin\angle A_2OM = \frac{MA_2}{OA_2}$$

$$or\ \ sin\frac{\pi}{n} = \frac{\left(\frac{a}{2}\right)}{OA_2} \qquad \Rightarrow OA_2 = \frac{a}{2}cosec\frac{\pi}{n} \qquad \left(\angle A_2OM = \frac{\pi}{n}\right)$$

In right ΔA_2OP (Fig. 1),

$$\Rightarrow \tan\angle OPA_2 = \frac{OA_2}{OP} \ \ or \quad \tan\beta = \frac{\left(\frac{a}{2}cosec\frac{\pi}{n}\right)}{H} \qquad \ldots\ldots\ldots\ldots..\ (IV)$$

On setting the value of H from eq(III) in the above eq(IV) as follows

$$\tan\beta = \frac{\left(\frac{a}{2}cosec\frac{\pi}{n}\right)}{\frac{a}{2}\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}}} = \frac{cosec\frac{\pi}{n}}{\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}}}$$

$$\Rightarrow \boldsymbol{cot\beta = sin\frac{\pi}{n}\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}}} \qquad \forall\left(0 \leq \alpha \leq \frac{2\pi}{n}\ \ \&\ \ 0 \leq\ \beta \leq \frac{\pi}{2}\right) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(V)$$

Above equation can be used to calculate the value of internal angle β if the face angle α & no. of sides 'n' are known without measuring the dimensions like normal height H & length of side a of the base.

2.2. Relation between angles $\boldsymbol{\alpha}$ & $\boldsymbol{\beta}$ for equally inclined 'n' no. of the straight-lines drawn from the single point in the space (Angle-Angle Relation)

Let there be 'n' no. of the straight-lines drawn from a single point (i.e. point of concurrency) in the space & are equally inclined at an angle $'\alpha'$ with one another in a consecutive manner such that the angle between any of n no. of lines & the axis symmetrically passing through the point of concurrency is $'\beta'$. (as shown in the figure 2 below) Now, this case becomes similar to that of a right pyramid with base as regular n-polygon. Thus, in this case α & β can also be co-related by eq(V) as follows

$$cot\beta = sin\frac{\pi}{n}\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}} \qquad (from\ the\ eq(V))$$

We can apply the conditions on the eq(V) to generalise it for n no. of the equally inclined straight lines drawn from a single point (i.e. point of concurrency) in the space as follows

$$\boldsymbol{if\ \alpha \to 0\ \Rightarrow \beta \to 0\quad \&\quad if\ \alpha = 0\ \Rightarrow \beta = 0}$$

$$\boldsymbol{if\ \alpha \to \frac{2\pi}{n} \Rightarrow \beta \to \frac{\pi}{2}\quad \&\quad if\ \alpha = \frac{2\pi}{n}\ \Rightarrow \beta = \frac{\pi}{2}}$$

By above conditions, both LHS & RHS are positive Hence, on squaring both the sides, we get

$$(cot\beta)^2 = \left(sin\frac{\pi}{n}\sqrt{cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}}\right)^2\quad or$$

$$cot^2\beta = sin^2\frac{\pi}{n}\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)$$

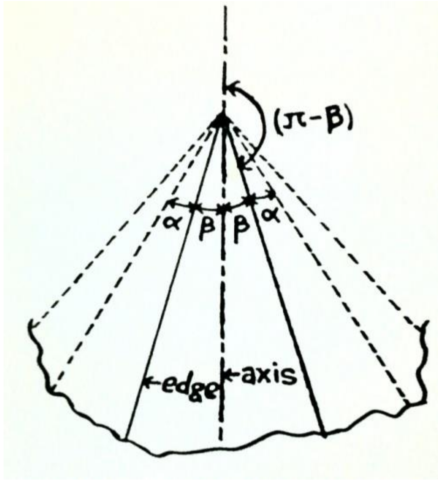

Figure 2: n no. of the concurrent straight lines or planes equally inclined with one another at an angle α.

$$\boldsymbol{cot^2\beta = sin^2\frac{\pi}{n}\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)}\quad \forall\left(0 \le \alpha \le \frac{2\pi}{n},\ 0 \le \beta \le \frac{\pi}{2}\ \ \&\ n \ge 3\right)\quad \ldots\ldots\ldots\ldots..(VI)$$

Above is the generalised formula to calculate the internal angle β of the geometrical axis with each of the lateral edges of a right pyramid having base as a regular polygon with n no. of sides each of equal length & an angle α between any two consecutive lateral edges. It's a dimensionless relation between the squares of angles α & β so is called Angle-Angle Relation. This is extremely useful to calculate the internal angle β or face angle α without measuring the normal height H or length a of the side of regular n-polygonal base. Moreover this formula can be applied on n no. of equally inclined planes intersecting each other at a single point in the space as well. It is very useful in 3D analysis of the angle between equally inclined straight lines & angle between the bonds in a molecule having regular tetrahedral structure etc.

2.3. Derivation of angle α by the symmetry of obliquity

For ease of calculations, let's consider $(n+1)$ no. of straight lines drawn from a single point in the space. Now, assume that one of the lines is fixed (as a reference line) & equally inclined at an angle α with all the rest n no. of lines which are themselves equally inclined at an angle α with one another in a consecutive manner.

Thus, this case becomes similar to the case of n no. of concurrent straight equally inclined at an angle $'\alpha'$ with one another in a consecutive manner such that the angle between any of n no. of lines & the axis (i.e. reference line) passing through point of concurrency is β (see the figure 2 above).

Hence, using the relation between $\boldsymbol{\alpha}$ & $\boldsymbol{\beta}$ from the eq(VI) as follows

$$cot^2\beta = sin^2\frac{\pi}{n}\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)$$

Applying above condition & setting $\pi - \beta = \alpha\ or\ \beta = \pi - \alpha$ in the above expression, we get

$$cot^2(\pi-\alpha) = sin^2\frac{\pi}{n}\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)\qquad \Rightarrow\ cot^2\alpha = sin^2\frac{\pi}{n}\left(cot^2\frac{\alpha}{2} - cot^2\frac{\pi}{n}\right)$$

$$\Rightarrow\ \frac{cos^2\alpha}{sin^2\alpha} = sin^2\frac{\pi}{n}\left(\frac{cos^2\frac{\alpha}{2}}{sin^2\frac{\alpha}{2}} - cot^2\frac{\pi}{n}\right)\ \Rightarrow \frac{cos^2\alpha}{sin^2\alpha} = sin^2\frac{\pi}{n}\left(\frac{cos^2\frac{\alpha}{2} - sin^2\frac{\alpha}{2}cot^2\frac{\pi}{n}}{sin^2\frac{\alpha}{2}}\right)$$

$$\Rightarrow\ cos^2\alpha sin^2\frac{\alpha}{2} = sin^2\alpha sin^2\frac{\pi}{n}\left(cos^2\frac{\alpha}{2} - sin^2\frac{\alpha}{2}cot^2\frac{\pi}{n}\right)$$

$$\Rightarrow\ \left(2cos^2\frac{\alpha}{2} - 1\right)^2\left(1 - cos^2\frac{\alpha}{2}\right) = (1 - cos^2\alpha)\left(sin^2\frac{\pi}{n}cos^2\frac{\alpha}{2} - \left(1 - cos^2\frac{\alpha}{2}\right)sin^2\frac{\pi}{n}cot^2\frac{\pi}{n}\right)$$

$$\left(since,\ \ cosA = 2cos^2\frac{A}{2} - 1\right)$$

$$\Rightarrow \left(4cos^4\frac{\alpha}{2} + 1 - 4cos^2\frac{\alpha}{2}\right)\left(1 - cos^2\frac{\alpha}{2}\right) = \left(1 - \left(2cos^2\frac{\alpha}{2} - 1\right)^2\right)\left(sin^2\frac{\pi}{n}cos^2\frac{\alpha}{2} - \left(1 - cos^2\frac{\alpha}{2}\right)cos^2\frac{\pi}{n}\right)$$

$$\Rightarrow 4cos^4\frac{\alpha}{2} + 1 - 4cos^2\frac{\alpha}{2} - 4cos^6\frac{\alpha}{2} - cos^2\frac{\alpha}{2} + 4cos^4\frac{\alpha}{2}$$
$$= \left(1 - 4cos^4\frac{\alpha}{2} - 1 + 4cos^2\frac{\alpha}{2}\right)\left(sin^2\frac{\pi}{n}cos^2\frac{\alpha}{2} - cos^2\frac{\pi}{n} + cos^2\frac{\alpha}{2}cos^2\frac{\pi}{n}\right)$$

$$\Rightarrow\ -4cos^6\frac{\alpha}{2} + 8cos^4\frac{\alpha}{2} - 5cos^2\frac{\alpha}{2} + 1 = \left(-4cos^4\frac{\alpha}{2} + 4cos^2\frac{\alpha}{2}\right)\left(cos^2\frac{\alpha}{2}\left(sin^2\frac{\pi}{n} + cos^2\frac{\pi}{n}\right) - cos^2\frac{\pi}{n}\right)$$

$$= \left(-4cos^4\frac{\alpha}{2} + 4cos^2\frac{\alpha}{2}\right)\left(cos^2\frac{\alpha}{2} - cos^2\frac{\pi}{n}\right)$$

$$\Rightarrow -4cos^6\frac{\alpha}{2} + 8cos^4\frac{\alpha}{2} - 5cos^2\frac{\alpha}{2} + 1 = -4cos^6\frac{\alpha}{2} + 4cos^4\frac{\alpha}{2} + 4cos^2\frac{\pi}{n}cos^4\frac{\alpha}{2} - 4cos^2\frac{\pi}{n}cos^2\frac{\alpha}{2}$$

$$\Rightarrow 4\left(1 - cos^2\frac{\pi}{n}\right)cos^4\frac{\alpha}{2} - \left(5 - 4cos^2\frac{\pi}{n}\right)cos^2\frac{\alpha}{2} + 1 = 0$$

$$or\qquad \left(4sin^2\frac{\pi}{n}\right)cos^4\frac{\alpha}{2} - \left(5 - 4cos^2\frac{\pi}{n}\right)cos^2\frac{\alpha}{2} + 1 = 0$$

Above equation is a quadratic equation in terms of $cos^2\,{}^{\alpha}/_{2}$. Hence, on solving the above equation, we have

$$cos^2\frac{\alpha}{2} = \frac{-\left(-\left(5 - 4cos^2\frac{\pi}{n}\right)\right) \pm \sqrt{\left(-\left(5 - 4cos^2\frac{\pi}{n}\right)\right)^2 - 4\left(4\left(1 - cos^2\frac{\pi}{n}\right)\right)(1)}}{2\left(4sin^2\frac{\pi}{n}\right)}$$

$$= \frac{\left(5 - 4cos^2\frac{\pi}{n}\right) \pm \sqrt{25 + 16cos^4\frac{\pi}{n} - 40cos^2\frac{\pi}{n} - 16 + 16cos^2\frac{\pi}{n}}}{8sin^2\frac{\pi}{n}}$$

$$= \frac{\left(5 - 4cos^2\frac{\pi}{n}\right) \pm \sqrt{16cos^4\frac{\pi}{n} - 24cos^2\frac{\pi}{n} + 9}}{8sin^2\frac{\pi}{n}}$$

$$= \frac{\left(5 - 4cos^2\frac{\pi}{n}\right) \pm \sqrt{\left(4cos^2\frac{\pi}{n}\right)^2 - 2\left(4cos^2\frac{\pi}{n}\right)(3) + 3^2}}{8sin^2\frac{\pi}{n}}$$

$$\boldsymbol{cos^2\frac{\alpha}{2} = \frac{\left(5 - 4cos^2\frac{\pi}{n}\right) \pm \sqrt{\left(3 - 4cos^2\frac{\pi}{n}\right)^2}}{8sin^2\frac{\pi}{n}}} \qquad \ldots\ldots\ldots\ldots\ldots\ (VII)$$

$$where\ \ \left(5 - 4cos^2\frac{\pi}{n}\right) > 0\ \ \&\ \left(1 - cos^2\frac{\pi}{n}\right) > 0\quad \forall\ n \in N$$

Above equation (VII) is called Characteristic Equation of Polyhedron with Angular Symmetry

$$where\ \left(3-4cos^2\frac{\pi}{n}\right)\ is\ called\ deterministic\ parameter\ of\ characteristic\ \ equation$$

Case 1:

$$\boldsymbol{if\ \left(3-4cos^2\frac{\pi}{n}\right)\geq 0}\ \Rightarrow\ 4cos^2\frac{\pi}{n}\leq 3\quad or\ \ cos^2\frac{\pi}{n}\leq\frac{3}{4}$$

$$\Rightarrow cos\frac{\pi}{n}\leq\frac{\sqrt{3}}{2}\quad or\ \ cos\frac{\pi}{n}\leq cos\frac{\pi}{6}\ \ \Rightarrow\ \frac{\pi}{n}\geq\frac{\pi}{6}\quad or\ \ n\leq 6$$

Hence the solution of eq(VII), considering only principal solution of trigonometric equation, is given as

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)\pm\left(3-4cos^2\frac{\pi}{n}\right)}{8sin^2\frac{\pi}{n}}$$

Taking positive sign,

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)+\left(3-4cos^2\frac{\pi}{n}\right)}{8sin^2\frac{\pi}{n}}=\frac{8-8cos^2\frac{\pi}{n}}{8sin^2\frac{\pi}{n}}=\frac{sin^2\frac{\pi}{n}}{sin^2\frac{\pi}{n}}=1\ \ \Rightarrow\ \frac{\alpha}{2}=0\ \ but\ \ \alpha\neq 0$$

Hence, **we discard this value of $\boldsymbol{\alpha}$**

Taking negative sign,

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)-\left(3-4cos^2\frac{\pi}{n}\right)}{8sin^2\frac{\pi}{n}}=\frac{2}{8sin^2\frac{\pi}{n}}=\frac{1}{4sin^2\frac{\pi}{n}}=\frac{cosec^2\frac{\pi}{n}}{4}$$

$$\Rightarrow\ cos\frac{\alpha}{2}=\frac{cosec\frac{\pi}{n}}{2}\quad\Rightarrow\boldsymbol{\alpha=2\cos^{-1}\left(\frac{1}{2}cosec\frac{\pi}{n}\right)}\qquad\forall\ \ \boldsymbol{3\leq n\leq 6}\quad(since,\ \ n\geq 3)\ \ \ldots\ldots..(VIII)$$

Hence**, we accept this value of $\boldsymbol{\alpha}$**

Case 2:

$$\boldsymbol{if\ \left(3-4cos^2\frac{\pi}{n}\right)<0}\ \Rightarrow\ 4cos^2\frac{\pi}{n}>3\quad or\ \ cos^2\frac{\pi}{n}>\frac{3}{4}$$

$$\Rightarrow cos\frac{\pi}{n}>\frac{\sqrt{3}}{2}\quad or\ \ cos\frac{\pi}{n}>cos\frac{\pi}{6}\ \ \Rightarrow\ \frac{\pi}{n}<\frac{\pi}{6}\quad or\ \ \boldsymbol{n>6}$$

Hence the solution of eq(VII), considering only principal solution of trigonometric equation, is given as

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)\pm\left(4cos^2\frac{\pi}{n}-3\right)}{8sin^2\frac{\pi}{n}}$$

Taking positive sign,

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)+\left(4cos^2\frac{\pi}{n}-3\right)}{8sin^2\frac{\pi}{n}}=\frac{2}{8sin^2\frac{\pi}{n}}=\frac{1}{4sin^2\frac{\pi}{n}}=\frac{cosec^2\frac{\pi}{n}}{4}$$

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$$\Rightarrow cos\frac{\alpha}{2}=\frac{cosec\frac{\pi}{n}}{2} \qquad \Rightarrow \boldsymbol{\alpha=2\cos^{-1}\left(\frac{1}{2}cosec\frac{\pi}{n}\right)}$$

$$but\ for\ existence\ of\ the\ above\ value\ of\ \alpha, \qquad we\ have\ the\ condition\ \ -1\leq\left(\frac{1}{2}cosec\frac{\pi}{n}\right)\leq 1$$

$$\Rightarrow \frac{1}{2}cosec\frac{\pi}{n}\leq 1 \quad (\ since, n\geq 3)$$

$$cosec\frac{\pi}{n}\leq 2\ or\ cosec\frac{\pi}{n}\leq cosec\frac{\pi}{6} \quad \Rightarrow \frac{\pi}{n}\geq\frac{\pi}{6} \Rightarrow \boldsymbol{n\leq 6}\ but\ we\ assumed\ \boldsymbol{n>6}$$

The above condition shows the contradiction i.e. it's against our assumption $n>6$ hence this value is discarded.

Taking negative sign,

$$cos^2\frac{\alpha}{2}=\frac{\left(5-4cos^2\frac{\pi}{n}\right)-\left(4cos^2\frac{\pi}{n}-3\right)}{8sin^2\frac{\pi}{n}}=\frac{2-8cos^2\frac{\pi}{n}}{8sin^2\frac{\pi}{n}}=\frac{1-4cos^2\frac{\pi}{n}}{4sin^2\frac{\pi}{n}}$$

$$but, we\ have\ a\ condition\ for\ real\ value\ of\ \alpha\ \Rightarrow\ 1-4cos^2\frac{\pi}{n}\geq 0$$

$$cos^2\frac{\pi}{n}\leq\frac{1}{4}\ \ or\ \ cos\frac{\pi}{n}\leq\frac{1}{2} \ \ \Rightarrow\ \ cos\frac{\pi}{n}\leq cos\frac{\pi}{3} \ \ \Rightarrow\frac{\pi}{n}\geq\frac{\pi}{3} \ \ \Rightarrow \ \ \boldsymbol{n\leq 3}\ \ but\ we\ assumed\ \boldsymbol{n\geq 3}$$

The above condition shows the contradiction i.e. it's against our assumption $n\geq 3$ hence this value is discarded.

2.4. Optimum solution for n no. of straight lines equally & adjacently inclined with each other

Acceptable solution for the value of α is given only from the eq(VIII) as follows

$$\alpha=2\cos^{-1}\left(\frac{1}{2}cosec\frac{\pi}{n}\right) \qquad \forall\ \ 3\leq n\leq 6$$

But if there is n no. of concurrent straight lines out of which $(n-1)$ lines are equally inclined with each other adjacently & with the reference line then the angle α is calculated by setting $n=(n-1)$ in above relation as follows

$$\alpha=2\cos^{-1}\left(\frac{1}{2}cosec\frac{\pi}{(n-1)}\right) \qquad \forall\ \ 3\leq(n-1)\leq 6$$

$$\Rightarrow\ \boldsymbol{\alpha=2\cos^{-1}\left\{\frac{1}{2}cosec\left(\frac{\pi}{n-1}\right)\right\}} \qquad \forall\ \ \boldsymbol{4\leq n\leq 7}\ \&\ \boldsymbol{n}\in\boldsymbol{N}$$

2.5. Important Deductions: Let's check out the values of angle α for different values of n & the corresponding cases as follows

Case 1: $n=4$: There are four straight lines equally inclined at an angle α with each other in the space i.e. they form a tetrahedral structure of four bonds (equally inclined with other in the space)).

$$\alpha = 2\cos^{-1}\left\{\frac{1}{2}cosec\left(\frac{\pi}{4-1}\right)\right\} = 2\cos^{-1}\left\{\frac{1}{2}\times\frac{2}{\sqrt{3}}\right\} = \mathbf{2\cos^{-1}\left\{\frac{1}{\sqrt{3}}\right\}}$$
$$\approx \mathbf{109.4712206^o \ or \ 109^o28'16.39''}$$

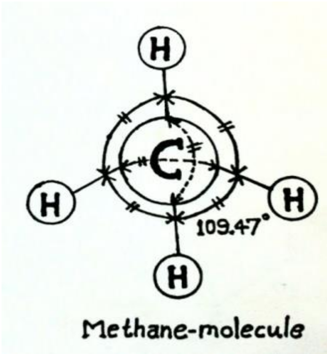

Figure 3. CH_4 **molecular structure.**

This case shows that all the four straight lines are equally inclined approximately at an angle of 109.47^o with each other in 3-D space. In this case, each straight line represents a bond in a regular tetrahedral structure hence it's true for any regular tetrahedral structure.

Eg: There are four σ-bonds of hydrogen atoms with a single centralised carbon atom which are equally inclined with each other in 3-D space hence assume four σ –bonds in CH_4 molecule as four straight lines equally inclined with each other in 3-D space. Thus, the angle between any two σ –bonds in CH_4 molecule is $\mathbf{109.47^o}$ as shown in the figures 2 & 3. Above value is the angle between any two σ-bonds in a molecule having a regular tetrahedral structure Eg. Methane Molecule (CH_4) (The case of $n = 4$ in the figure 4 below is indicating the angles of mutual inclination of bonds with each other in a regular tetrahedral structure).

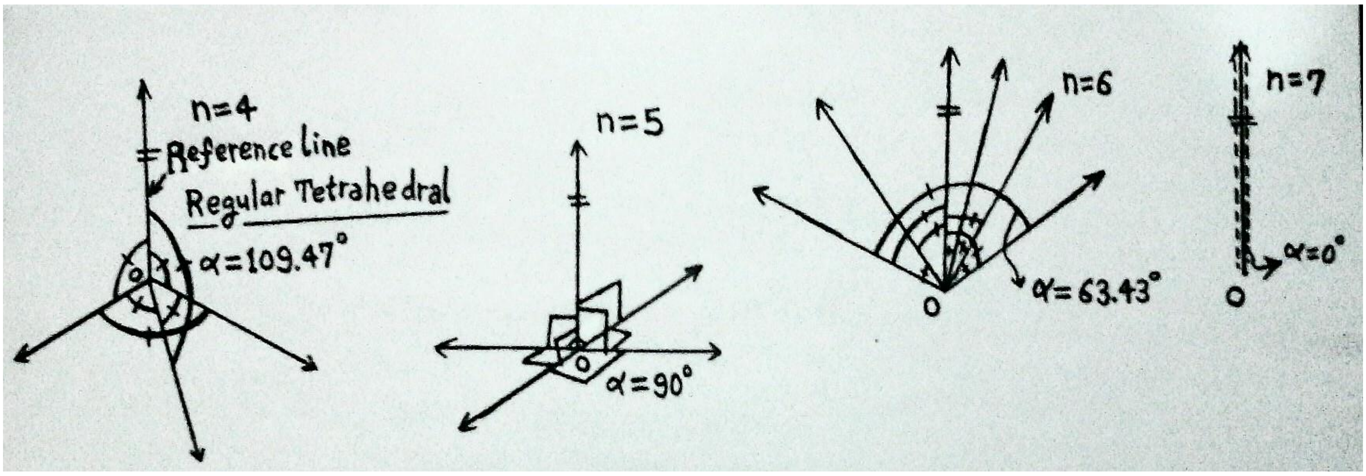

Figure 4: Different cases of configuration of equally inclined straight lines drawn from a single point in 3-D space.

Case 2: $\boldsymbol{n = 5}$: There are five straight lines out of which four lines are equally inclined with one another adjacently & with the fifth one (i.e. reference line) at the same angle α).

$$\alpha = 2\cos^{-1}\left\{\frac{1}{2}cosec\left(\frac{\pi}{5-1}\right)\right\} = 2\cos^{-1}\left\{\frac{1}{2}\times\sqrt{2}\right\} = \mathbf{2\cos^{-1}\left\{\frac{1}{\sqrt{2}}\right\}} = \mathbf{90^o}$$

The above value indicates that four straight lines out of five are co-planar making an angle 90^o with one another adjacently (same as the co-ordinate axes in X-Y plane) and with the fifth one (see the case of $n = 5$ in the figure 4 above).

Case 3: $\boldsymbol{n = 6}$: There are six straight lines out of which five lines are equally inclined with one another adjacently & with the sixth one (i.e. reference line) at the same angle α).

$$\alpha = 2\cos^{-1}\left\{\frac{1}{2}cosec\left(\frac{\pi}{6-1}\right)\right\} = 2\cos^{-1}\left\{\frac{1}{2}\times cosec36^o\right\} \approx \mathbf{63.43494882^o}$$

The above value indicates that five straight lines out of six are non- co-planar making an angle 63.43^o with one another adjacently and with the sixth one (see the case of $n = 6$ in the figure 4 above).

Case 4: $\boldsymbol{n = 7}$ **:** There are seven straight lines out of which six lines are equally inclined with one another adjacently & with the seventh one (i.e. reference line) at the same angle α).

$$\alpha = 2\cos^{-1}\left\{\frac{1}{2}cosec\left(\frac{\pi}{7-1}\right)\right\} = 2\cos^{-1}\left\{\frac{1}{2}\times 2\right\} = \mathbf{0^o}$$

The above value indicates that all the seven straight lines coincide with each other i.e. become a single straight line (see the case of $n = 7$ in the figure 4 above).

We, find that the case-1 is very important result used in analysis of tetrahedral voids in Solid State Physics.

3. Proof-2: Using HCR's dimensionless formula for regular n-polyhedron

We know that all the bonds of a molecule having a regular tetrahedral structure (ex. methane (CH_4) molecule) are equally inclined with each other in 3-D space. Thus, all these four bonds can be simply represented by the lateral edges of elementary right pyramids of a regular tetrahedron. Now, let the angle between any bonds in a tetrahedral structure be α then this angle α is also equal to the angle between any two consecutive lateral edges of the elementary right pyramid of a regular tetrahedral structure (see figure 5) hence it is easily found out by using HCR's formula [2] (used to calculate edge angle α of elementary right pyramid of any regular n-polyhedron) as follows

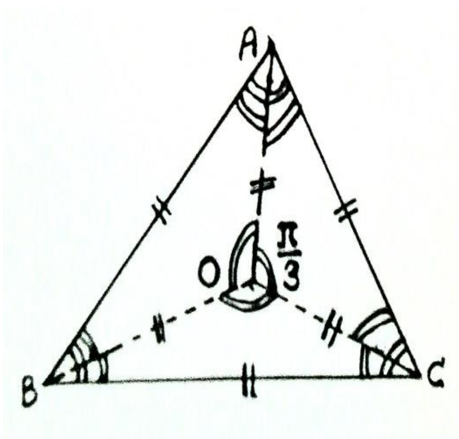

Figure 5: Regular Tetrahedron having four congruent equilateral triangular faces $(\boldsymbol{n = 3}\ \&\ \boldsymbol{n_f = 4})$.

$$\alpha = 2\tan^{-1}\left(sec\frac{\pi}{n}\sqrt{sin\left\{\frac{2\pi}{nn_f}\right\}sin\left\{\frac{2\pi(n_f-1)}{nn_f}\right\}}\right)$$

In this case of a regular tetrahedron, we have

$$n = no.of\ edges\ in\ one\ face = 3\ \ \&\ \ n_f = no.of\ faces = 4$$

Now, substituting these integer values in HCR's Formula, we get

$$\alpha = 2\tan^{-1}\left(sec\frac{\pi}{3}\sqrt{sin\left\{\frac{2\pi}{3\times 4}\right\}sin\left\{\frac{2\pi(4-1)}{3\times 4}\right\}}\right) = 2\tan^{-1}\left(sec\frac{\pi}{3}\sqrt{sin\left\{\frac{\pi}{6}\right\}sin\left\{\frac{\pi}{2}\right\}}\right)$$

$$= 2\tan^{-1}\left(2\sqrt{\frac{1}{2}\times 1}\right) = \mathbf{2\tan^{-1}(\sqrt{2})} \approx \mathbf{109.4712206^o}$$

The above value of edge angle (α) shows that the angle between any two bonds in a tetrahedral structure of molecule ex. methane (CH_4) is $2\tan^{-1}(\sqrt{2}) \approx 109.4712206^o \approx 109^o28'16.39''$.

Conclusion

In this work, the tetrahedral bond angle has been rigorously established using two independent geometric approaches, namely the analytical formulation of a right pyramid and the application of HCR's formula for regular polyhedra. In addition to confirming the tetrahedral structure, the analytic expressions derived here are useful for the structural analysis of right pyramids as well as regular and uniform polyhedra.

Note: Above articles had been derived *& illustrated by Mr H.C. Rajpoot (B Tech, Mechanical Engineering)*

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References

[1] Rajpoot CH. Advanced geometry. 1st ed. Chennai: Notion Press Media Pvt. Ltd.; 2013 Apr 3. ISBN: 97893-83808-15-1.

[2] Rajpoot HC. HCR's or H. Rajpoot's Formula for Regular Polyhedron. 2014.

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