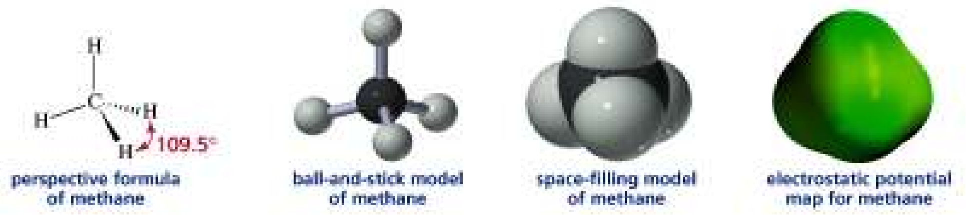
The optimal bond angle of Methane

1. Introduction

Methane 3-dimensional structure consists of 4 hydrogen atoms (H_1 , H_2, H_3, H_4) at the vertices of a regular tetrahedron (right pyramid) and 1 carbon (C) at the centre of the structure. We are interested in finding the optimal bond angle of $H_1 - C - H_2$ in this 3-dim structure. Reader may first read my article on a trigonometry solution that this angle is 109.5^{o}:

http://www.qc.edu.hk/math/Certificate%20Level/methane.htm



2. 3 – dimensional vector

I reconsider this problem a year after publishing the above web-page and come up with a better proof.

Let V be the centre of the tetrahedron, that is, the carbon atom.

Let A, B, C, D be the vertices, that is, the hydrogen atoms.

Let $|VA| = |VB| = |VC| = |VD| = R$

Let θ be bond angle.

By symmetry, $\overrightarrow{VA} + \overrightarrow{VB} + \overrightarrow{VC} + \overrightarrow{VD} = \vec{0}$

Consider the dot product : $\left(\overrightarrow{VA} + \overrightarrow{VB} + \overrightarrow{VC} + \overrightarrow{VD}\right) \bullet \left(\overrightarrow{VA} + \overrightarrow{VB} + \overrightarrow{VC} + \overrightarrow{VD}\right) = 0$ …. (1)

In the expansion of (1),

$$\overrightarrow{VA} \bullet \overrightarrow{VA} = \overrightarrow{VB} \bullet \overrightarrow{VB} = \overrightarrow{VC} \bullet \overrightarrow{VC} = \overrightarrow{VD} \bullet \overrightarrow{VD} = R^2 \quad \text{…. (2)}$$

and

$$\overrightarrow{VA} \bullet \overrightarrow{VB} = \overrightarrow{VB} \bullet \overrightarrow{VC} = \overrightarrow{VC} \bullet \overrightarrow{VD} = \overrightarrow{VD} \bullet \overrightarrow{VA} = \ldots = R^2 \cos\theta \quad \text{…. (3)}$$

Substitute (2), (3) in (1), $4R^2 + 2R^2 \cos\theta = 0$

$$\cos\theta = \frac{1}{3}$$

$$\theta \approx \underline{\underline{109.471^{\circ}}}$$