**Question**

A methane molecule has one carbon atom $C$ and four hydrogen atoms $H_1, H_2, H_3, H_4$. If we take the carbon atom to be centred at the origin $(0,0,0)$ then the hydrogen atoms $H_1, H_2, H_3, H_4$ have position vectors $R\hat{\mathbf{r}}_\mathbf{1}$, $R\hat{\mathbf{r}}_\mathbf{2}$, $R\hat{\mathbf{r}}_\mathbf{3}$, $R\hat{\mathbf{r}}_\mathbf{4}$ respectively, where $\mathbf{r_1} = \mathbf{i}+\mathbf{j}+\mathbf{k}$, $\mathbf{r_2} = -\mathbf{i}-\mathbf{j}+\mathbf{k}$, $\mathbf{r_3} = -\mathbf{i}+\mathbf{j}-\mathbf{k}$, $\mathbf{r_4} = \mathbf{i}-\mathbf{j}-\mathbf{k}$ and $R$ is a scalar known as the bond distance of the molecule. $R\hat{\mathbf{r}}_\mathbf{1}$, $R\hat{\mathbf{r}}_\mathbf{2}$, $R\hat{\mathbf{r}}_\mathbf{3}$, $R\hat{\mathbf{r}}_\mathbf{4}$ are called the bond vectors of the molecule.

**(a)** Calculate the unit vectors $\hat{\mathbf{r}}_\mathbf{1}$, $\hat{\mathbf{r}}_\mathbf{2}$, $\hat{\mathbf{r}}_\mathbf{3}$, $\hat{\mathbf{r}}_\mathbf{4}$ and hence write down the four bond vectors of the methane molecule.

**(b)** Find the angle between the bond vectors $R\hat{\mathbf{r}}_\mathbf{1}$ and $R\hat{\mathbf{r}}_\mathbf{2}$

**(c)** Calculate $R\hat{\mathbf{r}}_\mathbf{1}-R\hat{\mathbf{r}}_\mathbf{1}$ and hence express $|R\hat{\mathbf{r}}_\mathbf{1} - R\hat{\mathbf{r}}_\mathbf{1}|$, the distance between the hydrogen atoms $H_1$ and $H_2$, in terms of $R$.

**Answer**

**(a)** $|\mathbf{r}_i| = \sqrt{3}$ so we have the unit vectors:

$$\hat{\mathbf{r}}_1 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \hat{\mathbf{r}}_2 = \begin{pmatrix} -\frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \hat{\mathbf{r}}_3 = \begin{pmatrix} -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{pmatrix}, \quad \hat{\mathbf{r}}_4 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{pmatrix}$$

and the corresponding bond vectors:

$$R\hat{\mathbf{r}}_1 = \begin{pmatrix} \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix}, \quad R\hat{\mathbf{r}}_2 = \begin{pmatrix} -\frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix}, \quad R\hat{\mathbf{r}}_3 = \begin{pmatrix} -\frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \end{pmatrix}, \quad R\hat{\mathbf{r}}_4 = \begin{pmatrix} \frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \end{pmatrix}.$$

**(b)** Let $\theta$ be the angle between the bond vectors $R\hat{\mathbf{r}}_1$ and $R\hat{\mathbf{r}}_2$:

$$R\hat{\mathbf{r}}_1 \cdot R\hat{\mathbf{r}}_2 = \begin{pmatrix} \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix} \cdot \begin{pmatrix} -\frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix} = -\frac{R^2}{3} - \frac{R^2}{3} + \frac{R^2}{3} = -\frac{R^2}{3}$$

$|R\hat{\mathbf{r}}_1| = R, \quad |R\hat{\mathbf{r}}_2| = R$ so that:

$$\theta = \cos^{-1}\left(\frac{R\hat{\mathbf{r}}_1 \cdot R\hat{\mathbf{r}}_2}{|R\hat{\mathbf{r}}_1||R\hat{\mathbf{r}}_2|}\right) = \cos^{-1}\left(\frac{\frac{-R^2}{3}}{R^2}\right) = \cos^{-1}\left(\frac{-1}{3}\right) \approx 109.47°$$

**(c)**

$$R\hat{\mathbf{r}}_1 - R\hat{\mathbf{r}}_2 = \begin{pmatrix} \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix} - \begin{pmatrix} -\frac{R}{\sqrt{3}} \\ -\frac{R}{\sqrt{3}} \\ \frac{R}{\sqrt{3}} \end{pmatrix} = \begin{pmatrix} 2\frac{R}{\sqrt{3}} \\ 2\frac{R}{\sqrt{3}} \\ 0 \end{pmatrix}$$

so the distance between the atoms $H_1$ and $H_2$ is given by

$$\begin{aligned} |R\hat{\mathbf{r}}_1 - R\hat{\mathbf{r}}_2| &= \sqrt{\left(\frac{2R}{\sqrt{3}}\right)^2 + \left(\frac{2R}{\sqrt{3}}\right)^2 + 0} \\ &= \sqrt{\frac{8R^2}{3}} = 2R\sqrt{\frac{2}{3}} \end{aligned}$$