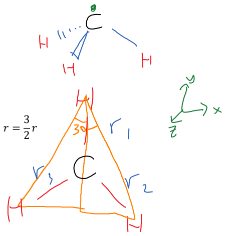
Methyl

Saturday, April 16, 2016 3:23 PM



$$\frac{1}{2}r + r = \frac{3}{2}r$$

$$\frac{3}{2}r = \sqrt{3}x$$
$$\frac{\sqrt{3}}{2}r = x$$

$$\vec{r_1} = \langle 0, r_{1,y}, r_{1,z}\rangle$$
$$\vec{r_2} = \langle r_{2,x}, r_{2,y}, r_{2,z}\rangle$$
$$\vec{r_3} = \langle r_{3,x}, r_{3,y}, r_{3,z}\rangle$$

$$r_{3,x} = -r_{2,x} = -x'_H$$
$$r_{2,y} = r_{3,y} = -y'_H$$
$$r_{1,z} = r_{2,z} = r_{3,z} = -z_H$$
$$r_{1,y} = \sqrt{{y'}_H^2 + {x'}_H^2}$$

$$\vec{r_1} = \langle 0, r_{x,y}, -r_z\rangle$$
$$\vec{r_2} = \left\langle \frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle$$
$$\vec{r_3} = \left\langle -\frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle$$

Check to see that all vectors are equal in length

$$|\vec{r_1}|^2 = \left(\sqrt{y^2 + x^2}\right)^2 + z^2 = x^2 + y^2 + z^2$$
$$|\vec{r_2}|^2 = |\vec{r_3}|^2 = x^2 + y^2 + z^2 = |\vec{r_1}|^2$$

The origin is at the Carbon
atom

Now that we have the relative positions of the atoms in CH_3 radical, we can now determine the total momentum, total angular momentum and center of mass

$$M = \sum_i^4 m_i = m_c + 3m_h$$

$$R_{CM} = \frac{1}{M}\sum_i^4 m_i r_i = \frac{1}{M}\left(m_c\vec{r_c} + m_h(\vec{r}_1 + \vec{r}_2 + \vec{r}_3)\right)$$

$$\vec{r}_c = 0$$

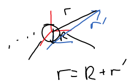
$$\vec{R}_{CM} = \frac{1}{M}\sum_i^4 m_i r_i = \frac{m_H}{m_c + 3m_h}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) = \frac{m_H}{m_c + 3m_h}\left(\langle 0, r_{x,y}, -r_z\rangle + \left\langle \frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle + \left\langle -\frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle\right)$$

$$= \frac{m_H}{m_C + 3m_H}\langle 0,0,-3r_z\rangle$$

$$\vec{R}_{CM} = \frac{m_H}{m_c + 3m_h}\langle 0,0,-3z_H\rangle = \alpha\langle 0,0,-3r_z\rangle$$

$$\alpha = \frac{m_H}{m_c + 3m_h}$$

$$m_H = 1.008u$$
$$m_C = 12.000u$$
$$\vec{R}_{cm} = \frac{1.008u}{12.000u + 3 * 1.008u}\langle 0,0,-3r_z\rangle = \langle 0,0,-3\alpha r_z\rangle$$



$$\vec{P} = \sum_i^4 m_i\dot{\vec{r}}_i$$

define new coordinate system S′ shifted to the the center of mass

$$\vec{L} = \sum_i^4 r_i \times m_i\dot{\vec{r}}_i = \vec{R}\times\vec{P} + \sum_i^4 \vec{r}_i' \times m_i\dot{\vec{r}}_i'$$

$$\vec{r}' = \vec{r} - R_{cm}$$

$$L = \vec{R}\times\vec{P} + \sum_i^4 m_i\left(\vec{r}_i' \times \vec{v}_i{}'\right)$$

$$m_i\left(\vec{r}_i - \vec{R}_{cm}\right)\times\left(\dot{\vec{r_i}} - \dot{\vec{R}}_{cm}\right)$$

$$\vec{r_1} = \langle 0, r_{x,y}, -r_z\rangle \Rightarrow, \qquad \vec{r}_1' = \langle 0, r_{x,y}, -r_z + 3\alpha r_z\rangle = \langle 0, r_{x,y}, r_z(3\alpha - 1)\rangle$$
$$\vec{r_2} = \left\langle \frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle \Rightarrow \qquad \vec{r}_2' = \left\langle \frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, r_z(3\alpha - 1)\right\rangle$$
$$\vec{r_3} = \left\langle -\frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, -r_z\right\rangle \Rightarrow \quad \vec{r}_3' = \left\langle -\frac{\sqrt{3}}{2}r_{x,y}, -\frac{1}{2}r_{x,y}, r_z(3\alpha - 1)\right\rangle$$
$$\vec{r}_c = \vec{r}_4 = 0 \qquad \Rightarrow \quad \vec{r}_4' = \langle 0,0,3\alpha r_z\rangle$$

Find a source for
atomic masses

$$L = \vec{R}\times\vec{P} + \sum_i^4 m_i\left(\vec{r}_i' \times \vec{v}_i{}'\right)$$

$$\vec{r}_i' \times \vec{v}_i' = \vec{r}_i' \times \vec{\omega}_i \times \vec{r}_i' = \vec{r}_i' \times \begin{vmatrix} i & j & k \\ \omega_x^i & \omega_y^i & \omega_z^i \\ r_x^{i'} & r_y^{i'} & r_z^{i'} \end{vmatrix}$$

$$\begin{vmatrix} i & j & k \\ \omega_x^i & \omega_y^i & \omega_z^i \\ r_x^i & r_y^i & r_z^i \end{vmatrix} = \left\langle \omega_y^i r_z^{i'} - \omega_z^i r_y^{i'}, -\left(\omega_x^i r_z^{i'} - \omega_z^i r_x^{i'}\right), \omega_x^i r_y^{i'} - \omega_y^i r_x^{i'}\right\rangle = \left\langle \omega_y^i r_z^{i'} - \omega_z^i r_y^{i'}, \omega_z^i r_x^{i'} - \omega_x^i r_z^{i'}, \omega_x^i r_y^{i'} - \omega_y^i r_x^{i'}\right\rangle$$

$$\begin{vmatrix} i & j & k \\ r_x^{i'} & r_y^{i'} & r_z^{i'} \\ \omega_y^i r_z^{i'} - \omega_z^i r_y^{i'} & \omega_z^i r_x^{i'} - \omega_x^i r_z^{i'} & \omega_x^i r_y^{i'} - \omega_y^i r_x^{i'} \end{vmatrix} = \begin{pmatrix} \omega_x^i r_y^{i'} r_y^{i'} - \omega_y^i r_x^{i'} r_y^{i'} - \omega_z^i r_x^{i'} r_z^{i'} + \omega_x^i r_z^{i'} r_z^{i'} \\ \omega_y^i r_z^{i'} r_z^{i'} - \omega_z^i r_y^{i'} r_z^{i'} - \omega_x^i r_y^{i'} r_x^{i'} + \omega_y^i r_x^{i'} r_x^{i'} \\ \omega_z^i r_x^{i'} r_x^{i'} - \omega_x^i r_z^{i'} r_x^{i'} - \omega_y^i r_z^{i'} r_y^{i'} + \omega_z^i r_y^{i'} r_y^{i'} \end{pmatrix} = \begin{pmatrix} \omega_x^i\left[\left(r_y^{i'}\right)^2 + \left(r_z^{i'}\right)^2\right] - \omega_y^i r_x^{i'} r_y^{i'} - \omega_z^i r_x^{i'} r_z^{i'} \\ \omega_y^i\left[r_z^{i'} r_z^{i'} + r_x^{i'} r_x^{i'}\right] - \omega_z^i r_y^{i'} r_z^{i'} - \omega_x^i r_y^{i'} r_x^{i'} \\ \omega_z^i\left[r_x^{i'} r_x^{i'} + r_y^{i'} r_y^{i'}\right] - \omega_x^i r_z^{i'} r_x^{i'} - \omega_y^i r_z^{i'} r_y^{i'} \end{pmatrix} = m\begin{pmatrix} \left[\left(r_y'\right)^2 + (r_z')^2\right] & -r_x' r_y' & -r_x' r_z' \\ -r_x' r_y' & [(r_z')^2 + (r_x')^2] & -r_y' r_z' \\ -r_x' r_z' & -r_y' r_z' & \left[(r_x')^2 + \left(r_y'\right)^2\right] \end{pmatrix}\begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

$$L = \vec{R}\times\vec{P} + \sum_i^4 m_i \begin{pmatrix} \left[\left(r_y'\right)^2 + (r_z')^2\right] & -r_x' r_y' & -r_x' r_z' \\ -r_x' r_y' & [(r_z')^2 + (r_x')^2] & -r_y' r_z' \\ -r_x' r_z' & -r_y' r_z' & \left[(r_x')^2 + \left(r_y'\right)^2\right] \end{pmatrix}_i \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}_i$$

$$I_{xx} = \sum_i^4 m_i\left(r_y^{2'} + r_z^{2'}\right)_i, \qquad I_{xy} = I_{yx} = -\sum m_i(xy)_i$$
$$I_{yy} = \sum_i^4 m_i\left(r_x^{2'} + r_z^{2'}\right)_i, \qquad I_{xz} = I_{zx} = -\sum m_i(xz)_i$$
$$I_{zz} = \sum_i^4 m_i\left(r_x^{2'} + r_y^{2'}\right)_i, \qquad I_{yz} = I_{yz} = -\sum m_i(yz)_i$$

Diagonal Elements

$$I_{xx} = \sum_i^4 m_i\left(r_y^{2'} + r_z^{2'}\right)_i = m_c(3\alpha r_z)^2 + m_H\left[\left(r_{x,y}^2 + r_z^2(3\alpha - 1)^2\right) + 2\left(\frac{r_{x,y}^2}{4} + r_z^2(3\alpha - 1)^2\right)\right] = m_c(3\alpha r_z)^2 + m_H\left[\left(\frac{3r_{x,y}^2}{2}\right) + 3r_z^2(3\alpha - 1)\right]$$

$$I_{yy} = \sum_i^4 m_i\left(r_x^{2'} + r_z^{2'}\right)_i = m_c(3\alpha r_z)^2 + m_H\left[r_z^2(3\alpha - 1)^2 + 2\left(\frac{3}{4}r_{x,y} + r_z^2(3\alpha - 1)^2\right)\right] = m_c(3\alpha r_z)^2 + m_H\left[3r_z^2(3\alpha - 1)^2 + \frac{3}{2}r_{x,y}^2\right]$$

$$I_{zz} = \sum_i^4 m_i\left(r_x^{2'} + r_y^{2'}\right)_i = m_c * 0 + m_H\left[0^2 + r_{x,y}^2 + 2\left(\frac{3}{4}r_{x,y}^2 + \frac{1}{4}r_{x,y}^2\right)\right] = 3m_H\left[r_{x,y}^2\right]$$

$$I_{xx} = I_{yy} = m_c(3\alpha r_z)^2 + m_H\left[3r_z^2(3\alpha - 1)^2 + \frac{3}{2}r_{x,y}^2\right], \qquad I_{zz} = 3m_H\left[r_{x,y}^2\right]$$

Off Diagonal Elements

$$I_{xy} = I_{yx} = -\sum m_i(xy)_i = -\left[m_c * 0 * 0 + m_H\left(r_{x,y} * 0 + \frac{\sqrt{3}}{2}r_{x,y} * \left(-\frac{1}{2}r_{x,y}\right) + \frac{\sqrt{3}}{2}r_{x,y} * \left(\frac{1}{2}r_{x,y}\right)\right)\right] = 0$$

$$I_{xz} = I_{zx} = -\sum m_i(xz)_i = -\left|m_c(0 * 3\alpha r_z) + m_H\left[(0)r_z(3\alpha - 1) + \frac{\sqrt{3}}{2}r_{x,y}r_z(3\alpha - 1) - \frac{\sqrt{3}}{2}r_{x,y}r_z(3\alpha - 1)\right]\right| = 0$$

$$I_{yz} = I_{yz} = -\sum m_i(yz)_i = -\left[m_c(0)(3\alpha r_z) + m_H\left[r_{x,y}r_z(3\alpha - 1) - \frac{1}{2}r_{x,y}r_z(3\alpha - 1) - \frac{1}{2}r_{x,y}r_z(3\alpha - 1)\right]\right] = 0$$

$$I_{ij} = \begin{bmatrix} m_c(3\alpha r_z)^2 + m_H\left[\left(\frac{3r_{x,y}^2}{2}\right) + 3r_z^2(3\alpha - 1)\right] & 0 & 0 \\ 0 & m_c(3\alpha r_z)^2 + m_H\left[3r_z^2(3\alpha - 1)^2 + \frac{3}{2}r_{x,y}^2\right] & 0 \\ 0 & 0 & 3m_H\left[r_{x,y}^2\right] \end{bmatrix}$$

Feedback Signal: $u(t)$
Error Signal: $\epsilon(t)$

$$u(t) = K_{pro}\epsilon(t) + K_{int}\int \epsilon(t)\,dt$$

$$I_a = I_b = m_c(3\alpha r_z)^2 + m_H\left[3r_z^2(3\alpha - 1)^2 + \frac{3}{2}r_{x,y}^2\right], \qquad I_c = 3m_H\left[r_{x,y}^2\right]$$

$$I_{ij} = \begin{bmatrix} I_a & 0 & 0 \\ 0 & I_b & 0 \\ 0 & 0 & I_c \end{bmatrix}, \textit{this is a Oblate Symmetric Top}$$

$$L_i = I_{ij}\omega_j$$

$$L_{ij} = \begin{bmatrix} I_a & 0 & 0 \\ 0 & I_b & 0 \\ 0 & 0 & I_c \end{bmatrix}\begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 = I_a^2\omega_x^2 + I_b^2\omega_y^2 + I_c^2\omega_z^2 \Rightarrow L^2 - L_z^2 = L_x^2 + L_y^2$$

$$\hat{H}_{rot} = \frac{L_x^2}{2I_a} + \frac{L_y^2}{2I_b} + \frac{L_z^2}{2I_c} = \frac{L_x^2}{2I_a} + \frac{L_y^2}{2I_a} + \frac{L_z^2}{2I_c} = \frac{1}{2I_a}\left(L_x^2 + L_y^2\right) + \frac{L_z^2}{2I_c}$$

$$H_{rot} = \frac{L^2 - L_z^2}{2I_a} + \frac{L_z^2}{2I_c} \Rightarrow_{\left\{\begin{smallmatrix} switch \\ to \\ operators \end{smallmatrix}\right\}} \hat{H}_{rot} = \frac{\hat{L}^2 - \hat{L}_z^2}{2I_a} + \frac{\hat{L}_z^2}{2I_c}$$

$$\hat{L}^2|J,K\rangle = \hbar^2\big(J(J+1)\big)|J,K\rangle$$

$$\hat{L}_z^2|J,K\rangle = \hbar^2 K^2|J,K\rangle$$

$$\hat{H}_{rot}|J,K\rangle = E|J,K\rangle = \left(\frac{\hat{L}^2 - \hat{L}_z^2}{2I_a} + \frac{\hat{L}_z^2}{2I_c}\right)|J,K\rangle = \left(\frac{\hbar^2[J(J+1) - K^2]}{2I_a} + \frac{\hbar^2 K^2}{2I_c}\right)|J,K\rangle$$

$$E(J,K) = \frac{\hbar^2[J(J+1) - K^2]}{2I_a} + \frac{\hbar^2 K^2}{2I_c} = \frac{\hbar^2}{2I_a}(J(J+1) + \frac{\hbar^2 K^2}{2}\left(\frac{I}{I_c} - \frac{1}{I_a}\right) = \frac{\hbar^2}{2I_a}(J(J+1) + \frac{\hbar^2 K^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$E(J,K) = \frac{\hbar^2}{2I_a}\big(J(J+1)\big) + \frac{\hbar^2 K^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$E(J = J' + 1, K'') - E(J = J', K') = \Delta E(\Delta J = 1, \Delta K)$$

$$E(J = J' + 1, K'') = \frac{\hbar^2}{2I_a}\big((J' + 1)(J' + 1 + 1)\big) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) = \frac{\hbar^2}{2I_a}\big((J' + 1)(J' + 2)\big) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$= \frac{\hbar^2}{2I_a}\left(J'^2 + 3J' + 2\right) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$E(J = J' + 1, K'') - E(J = J', K') = \Delta E(\Delta J = 1, \Delta K)$$

$$E(J', K') = \frac{\hbar^2}{2I_a}\big(J'(J' + 1)\big) + \frac{\hbar^2 K'^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) = \frac{\hbar^2}{2I_a}\left(J'^2 + J'\right) + \frac{\hbar^2 K'^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$\Delta E_{rot}(\Delta J = 1, \Delta K) = \frac{\hbar^2}{2I_a}\left(J'^2 + 3J' + 2\right) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) - \frac{\hbar^2}{2I_a}\left(J'^2 + J'\right) - \frac{\hbar^2 K'^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$= \frac{\hbar^2}{2I_a}\left(J'^2 + 3J' + 2 - J'^2 - J'\right) + \frac{\hbar^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)\left(K''^2 - K'^2\right)$$

$$\Delta E_{rot}(\Delta J = 1, \Delta K) = \frac{\hbar^2}{I_a}(J' + 1) + \frac{\hbar^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)\left(K''^2 - K'^2\right)$$

$$\Delta E_{rot}(\Delta J = 0, \Delta K) = \frac{\hbar^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)\left(K''^2 - K'^2\right)$$

$$\Delta E_{rot}(\Delta J = -1, \Delta K) = E(J = J' - 1, K'') - E(J = J', K')$$

$$E(J = J' - 1, K'') = \frac{\hbar^2}{2I_a}\big((J' - 1)(J' - 1 + 1)\big) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) = \frac{\hbar^2}{2I_a}\big((J' - 1)(J')\big) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) = \frac{\hbar^2}{2I_a}\left(J'^2 - J'\right) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$E(J', K') = \frac{\hbar^2}{2I_a}\big(J'(J' + 1)\big) + \frac{\hbar^2 K^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) = \frac{\hbar^2}{2I_a}\left(J'^2 + J'\right) + \frac{\hbar^2 K'^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$\Delta E_{rot}(\Delta J = -1, \Delta K) = \frac{\hbar^2}{2I_a}\left(J'^2 - J'\right) + \frac{\hbar^2 K''^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right) - \frac{\hbar^2}{2I_a}\left(J'^2 + J'\right) - \frac{\hbar^2 K'^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$= \frac{\hbar^2}{2I_a}\left(J'^2 - J' - J'^2 - J'\right) + \frac{\hbar^2\left(K''^2 - K'^2\right)}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$= \frac{\hbar^2}{2I_a}(-2J') + \frac{\hbar^2\left(K''^2 - K'^2\right)}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)$$

$$= \frac{\hbar^2}{I_a}(J') + \frac{\hbar^2}{2}\left(\frac{I_a - I_c}{I_a I_c}\right)\left(K''^2 - K'^2\right)$$

$$\begin{bmatrix} 2 & 6 & 10 & 14 & 18 \\ 2 & 6 & 10 & 14 & 18 \\ 1 & 3 & 5 & 7 & 9 \\ 2 & 6 & 10 & 14 & 18 \\ 2 & 6 & 10 & 14 & 18 \end{bmatrix}$$