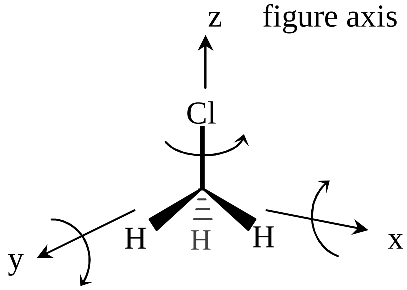
<u>Rotational Spectroscopy- Symmetric Tops</u>

Classical:

$$E = \frac{J_x^2}{2I_{xx}} + \frac{J_y^2}{2I_{yy}} + \frac{J_z^2}{2I_{zz}}$$



$I_{yy} = I_{xx} = I_\perp$ $\qquad$ $I_{zz} = I_\|$

$$E = \frac{1}{2I_\perp}(J_x^2 + J_y^2) + \frac{1}{2I_\|} J_z^2$$

$$E = \frac{1}{2I_\perp}(J_x^2 + J_y^2) + \frac{1}{2I_\perp} J_z^2 + \frac{1}{2I_\|} J_z^2 - \frac{1}{2I_\perp} J_z^2$$

$$E = \frac{J^2}{2I_\perp} + \left(\frac{1}{2I_\|} - \frac{1}{2I_\perp}\right) J_z^2 \qquad J^2 = J_x^2 + J_y^2 + J_z^2$$

$J^2 = \hbar^2 J(J+1)$ $\qquad$ $J_z = K\hbar$ $\qquad$ $K = 0, \pm1, \pm2, ..., \pm J$

$$\tilde{F}_{JK} = \tilde{B}J(J+1) + (\tilde{A} - \tilde{B})K^2$$

$$\tilde{B} = \frac{\hbar}{4\pi I_\perp c} \qquad \tilde{A} = \frac{\hbar}{4\pi I_\| c}$$

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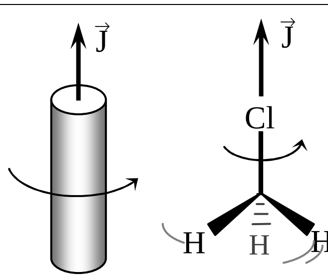
dipole moment parallel to figure axis ($\approx$ handle)

$\Delta K = 0$ $\qquad$ $\Delta J = \pm 1$

$$\tilde{\nu}_J = \tilde{F}_{J',K} - \tilde{F}_{J'-1,K} = \tilde{B}J(J+1) - \tilde{B}(J-1)(J-1+1)$$

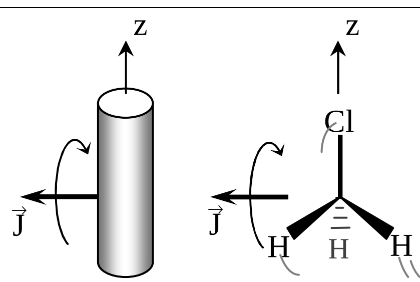
$= 2\tilde{B}J'$ $\qquad$ as for diatomics

J' ~ upper level



J = K

no change in electric
field as molecule rotates



K = 0