# Calculation of the Moment of Inertia for Polyatomic Molecules

Let: $(x_i, y_i, z_i)$ be the set of coordinates of all atoms in the molecule
$(\bar{x}, \bar{y}, \bar{z})$ be the coordinates of the center of mass of the molecule

Then:
$$I_{xx} = \sum m_i (y_i - \bar{y})^2 + \sum m_i (z_i - \bar{z})^2$$
$$I_{yy} = \sum m_i (x_i - \bar{x})^2 + \sum m_i (z_i - \bar{z})^2$$
$$I_{zz} = \sum m_i (x_i - \bar{x})^2 + \sum m_i (y_i - \bar{y})^2$$
$$I_{xy} = I_{yx} = \sum m_i (x_i - \bar{x})(y_i - \bar{y})$$
$$I_{xz} = I_{zx} = \sum m_i (z_i - \bar{z})(x_i - \bar{x})$$
$$I_{yz} = I_{zy} = \sum m_i (z_i - \bar{z})(y_i - \bar{y})$$

$$\overline{\overline{I}} = \begin{vmatrix} I_{xx} & -I_{yx} & -I_{zx} \\ -I_{xy} & I_{yy} & -I_{zy} \\ -I_{xz} & -I_{yz} & I_{zz} \end{vmatrix} = \begin{vmatrix} I_x & 0 & 0 \\ 0 & I_y & 0 \\ 0 & 0 & I_z \end{vmatrix}$$

Where: $I_x$, $I_y$, and $I_z$ are the principle axes of inertia

Thus: $I_x I_y I_z = \det(\overline{I}) = I_{xx}I_{yy}I_{zz} - I_{zz}I_{xy}^{\,2} - I_{xx}I_{yz}^{\,2} - I_{yy}I_{xz}^{\,2} - 2I_{xy}I_{xz}I_{yz}$

and the product $I_x I_y I_z$ is all we need to compute:

$$q_r = \frac{\pi^{1/2}}{\sigma}\left(\frac{8\pi^2 kT}{h^2}\right)^{3/2}\left(I_A I_B I_C\right)^{1/2}$$