

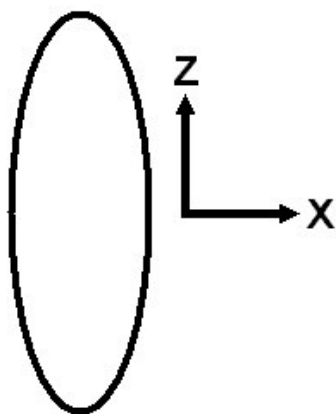
The Alignment Frame within the Molecule

Three orthogonal axes:

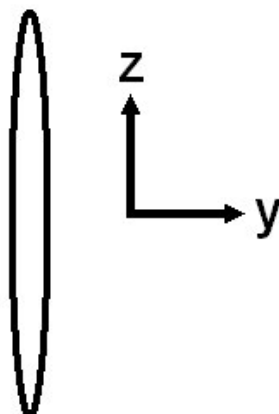
The long (z) axis: $\langle 3\cos^2\Theta_z - 1 \rangle = D_{zz}$

The “medium” (x) axis: $\langle 3\cos^2\Theta_x - 1 \rangle = D_{xx}$

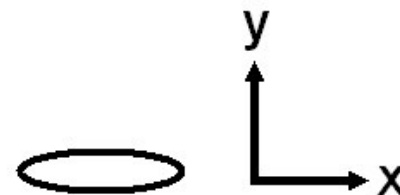
The short (y) axis: $\langle 3\cos^2\Theta_y - 1 \rangle = D_{yy}$



Side View



Side View



Top View