

Predicting the Value of the Residual Dipolar Coupling, D

- In the Alignment Frame, Polar coordinates can be used to describe the orientation of the N-H vector:

$$D = D_a \left\{ \begin{array}{l} (3\cos^2\Theta - 1) \\ + \frac{3}{2} R(\sin^2\Theta \cos 2\Phi) \end{array} \right\}$$

(2 to -1) (1 to -1)

where $D_a = 1/3 [D_{zz} - (D_{xx} + D_{yy})/2]$ is a measure of the degree of alignment

and $R = 1/3 (D_{xx} - D_{yy}) / D_a$ is a measure of the rhombicity (deviation from axial symmetry)