RIGID ROTOR WAVEFUNCTIONS **Chemistry BC3253x**

UNNORMALIZED CONTRIBUTIONS to SPHERICAL HARMONICS

$$Y_{J,M}(\theta,\varphi) = N_{J,M}\,\Theta(\theta)\,\Phi(\varphi)$$

J	M	$\Theta(\theta)$	$\Phi(\varphi)$
0	0	1	1
1	0	$\cos\theta$	1
1	± 1	$\sin\theta$	$e^{\pm iM\varphi}$
2	0	$(1/2)(3\cos^2\theta - 1)$	1
2	± 1	$\sin\theta\cos\theta$	$e^{\pm iM\varphi}$
2	± 2	$\sin^2\theta$	$e^{\pm 2iM\varphi}$
3	0	$(1/2)(5\cos^3\theta - 3\cos\theta)$	1
3	± 1	$(3/2)(\sin\theta)(5\cos^2\theta - 1)$	$e^{\pm iM\varphi}$
3	± 2	$15\cos\theta\sin^2\theta$	$e^{\pm 2iM\varphi}$
3	± 3	$15\sin^3\theta$	$e^{\pm 3iM\varphi}$

NORMALIZATION: $d\tau = \sin\theta\, d\theta\, d\varphi$; θ **from 0 to** π; φ **from 0 to** 2π

$$N_{J,M}^2 \int_0^{2\pi} \int_0^{\pi} Y_{J,M}^* \, Y_{J,M} \sin\vartheta \, d\vartheta \, d\varphi = 1$$

$$\int_0^{2\pi} \int_0^{\pi} Y_{J,M}^* \, Y_{J,M} \sin\vartheta \, d\vartheta \, d\varphi = \int_0^{2\pi} \Phi_M^* \, \Phi_M \, d\varphi \int_0^{\pi} \Theta_{J,M}^* \, \Theta_{J,M} \sin\vartheta \, d\vartheta$$

$$\int_0^{2\pi} \Phi_M^* \, \Phi_M \, d\varphi \int_0^{\pi} \Theta_{J,M}^* \, \Theta_{J,M} \sin\vartheta \, d\vartheta = 2\pi \int_0^{\pi} \Theta_{J,M}^* \, \Theta_{J,M} \sin\vartheta \, d\vartheta$$

i.e. the normalization for $\Phi_M(\varphi)$ is always $(2\pi)^{-1/2}$

J=0: $\int_0^{\pi} \Theta_{J,M}^* \, \Theta_{J,M} \sin\vartheta \, d\vartheta = \int_0^{\pi} \sin\vartheta \, d\vartheta = 2$ i.e. $N_{0,0} = 1/\sqrt{4\pi}$