

Gaussian Basis Functions (Cartesian Gaussians)

$$g_A = N(x - x_A)^k (y - y_A)^l (z - z_A)^m e^{-\alpha(\vec{r} - \vec{A})^2}$$

$$g_{s,A} = \left(\frac{2\alpha}{\pi} \right)^{3/4} e^{-\alpha r_A^2}$$

$$g_{p_x,A} = \left(\frac{2\alpha}{\pi} \right)^{3/4} 2\sqrt{\alpha} x_A e^{-\alpha r_A^2} = 2\sqrt{\alpha} x_A g_{s,A}$$

⋮

$$g_{p_z,A} = \left(\frac{2\alpha}{\pi} \right)^{3/4} 2\sqrt{\alpha} z_A e^{-\alpha r_A^2} = 2\sqrt{\alpha} z_A g_{s,A}$$

$$g_{d_{xy},A} = \left(\frac{2\alpha}{\pi} \right)^{3/4} 4\sqrt{\alpha} x_A y_A e^{-\alpha r_A^2} = 4\alpha x_A y_A g_{s,A}$$

$$g_{d_{x^2},A} = \left(\frac{2\alpha}{\pi} \right)^{3/4} \frac{4\alpha}{\sqrt{3}} x_A^2 e^{-\alpha r_A^2} = \frac{4\alpha}{\sqrt{3}} x_A^2 g_{s,A}$$

Note: No basis function has a radial node except at 0 and ∞