

1 Problem 1

The d orbitals have the nomenclature d_{z^2} , d_{xy} , d_{xz} , d_{yz} , and $d_{x^2-y^2}$. Show how the d orbital given below can be written in the form $y z F(r)$.

$$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81 \sqrt{\pi}} \left(\frac{1}{a_o} \right)^{3/2} \frac{r^2}{a_o^2} e^{-r/3a_o} \sin(\theta) \cos(\theta) \sin(\phi)$$

1.1 Solution

$$\begin{aligned} z &= r \cos(\theta) \\ x &= r \sin(\theta) \cos(\phi) \\ y &= r \sin(\theta) \sin(\phi) \end{aligned}$$

Thus,

$$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81 \sqrt{\pi}} \left(\frac{1}{a_o} \right)^{3/2} \frac{r^2}{a_o^2} e^{-r/3a_o} \sin(\theta) \cos(\theta) \sin(\phi)$$

$$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81 \sqrt{\pi}} \left(\frac{1}{a_o} \right)^{3/2} \frac{1}{a_o^2} e^{-r/3a_o} \left(\underbrace{r \sin(\theta) \sin(\phi)}_{\mathbf{y}} \right) \left(\underbrace{r \cos(\theta)}_{\mathbf{z}} \right)$$

$$\psi_{3d_{yz}} = F(r) y z$$