

# 1 Cognitive reasoning in the chemical sciences 3.5

## 1.1 Atomic and molecular orbitals

### 1. Drawing atomic orbitals as contour maps

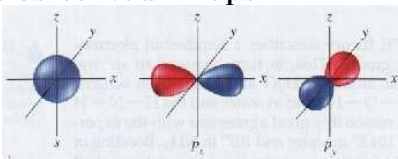


Figure 1: The three  $p$ -orbitals

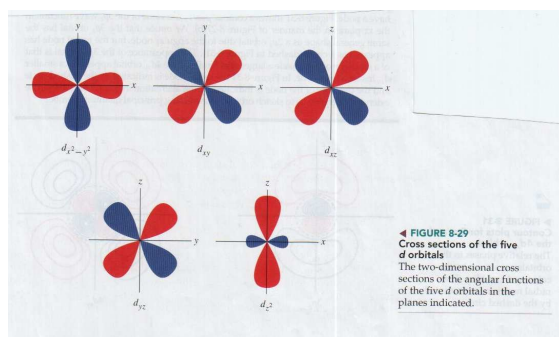


Figure 2: The five  $d$ -orbitals

- Describe the spatial points which fulfill the equation  $x = 0$ ?
  - Describe the spatial points which fulfill the equation  $xy = 0$ ?
  - Describe the spatial points which fulfill the equation  $x^2 - y^2 = 0$ ?
  - Describe the spatial points which fulfill the equation  $2z^2 - x^2 - y^2 = 0$ ? Strange but true fact: chemists abbreviate this function as  $z^2$ .
  - Please draw as a contour map the  $2p_z$  orbital for the  $x = 0$  plane.
  - Please draw as a contour map the  $2p_z$  orbital passing for the  $z = 0.5 \text{ \AA}$  plane.
  - Please draw as a contour map the three  $sp^2$  orbitals shown above passing for the  $z = 0.0$  plane.
  - Please draw as a contour map the  $3d_{xy}$  orbital passing through the  $z = 0$  plane.
  - Please draw as a contour map the  $3d_{xz}$  orbital passing through the  $z = 0$  plane.
  - Please draw as a contour map the  $3d_{x^2-y^2}$  orbital passing through the  $z = 0$  plane.
  - Please draw as a contour map the  $4p_z$  orbital passing through the  $x - z = 0$  plane.
2. Using contour maps to sharpen our understanding of previous things we have studied:
- Find in the diagram below the bongo drum modes corresponding to a  $3p$  state. Please draw this state as a drum mode. Note the outermost circles in the pictures represent the edge of the drum: they are not nodes.

- (b) Find in the diagram below the bongo drum modes corresponding to a 4d state. Please draw this state as a contour map. Note the outermost circles in the pictures represent the edge of the drum: they are not nodes.

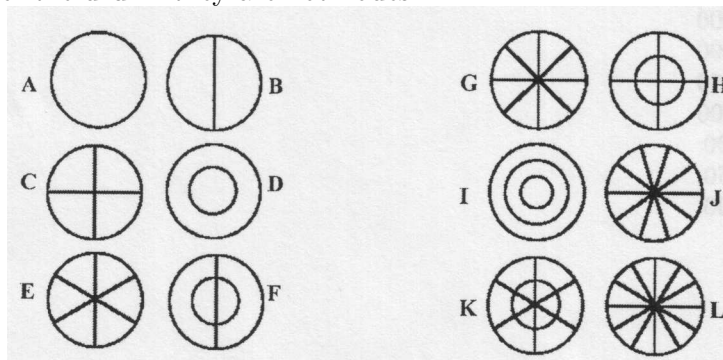


Figure 3: Nodal patterns for both bongo and kettle drums

- (c) Draw a contour map for a hydrogen  $3p_x$  orbital in the  $z = 0$  plane using the information contained in the radial distribution functions shown below.
- (d) Draw a contour map for a hydrogen  $3s$  orbital in the  $z = 0$  plane using the information contained in the radial distribution functions shown below.

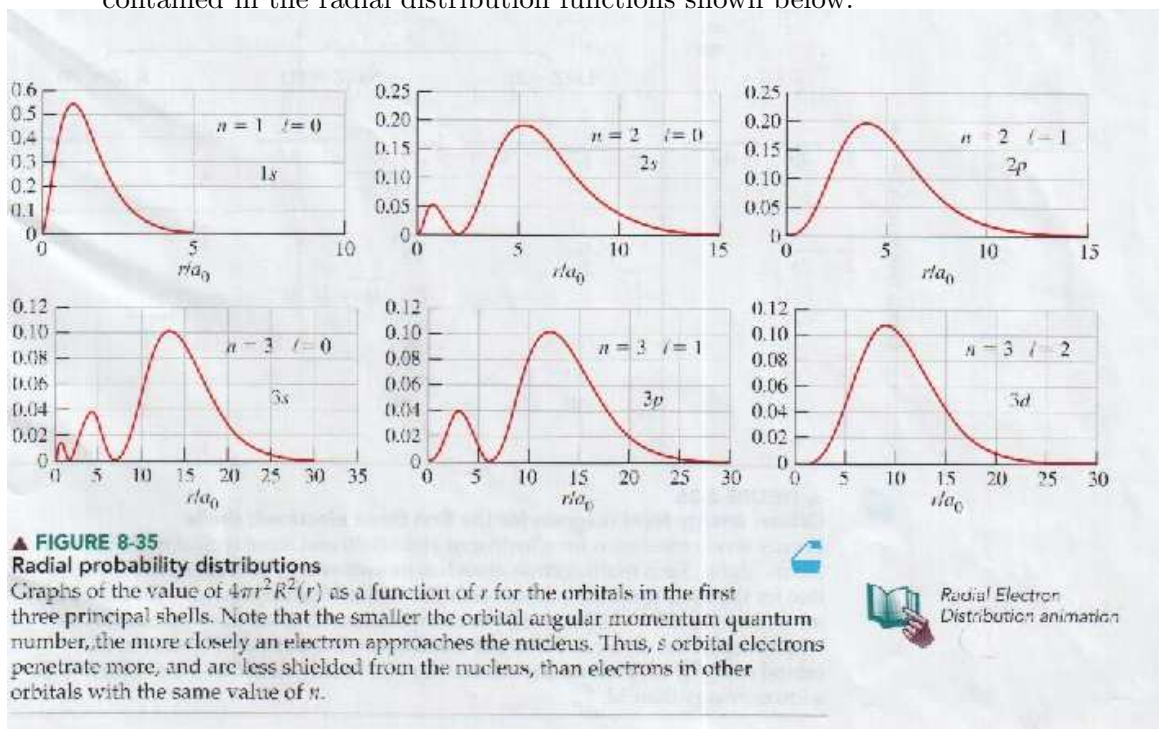


Figure 4: Radial distribution functions for the H atom

- (e) Indicate with a pair of qualitative contour maps what happens to the  $2s$  orbital in the  $\text{He}^+$  ion vs. the H ion. What is  $Z_{eff}$  for the helium cation?