

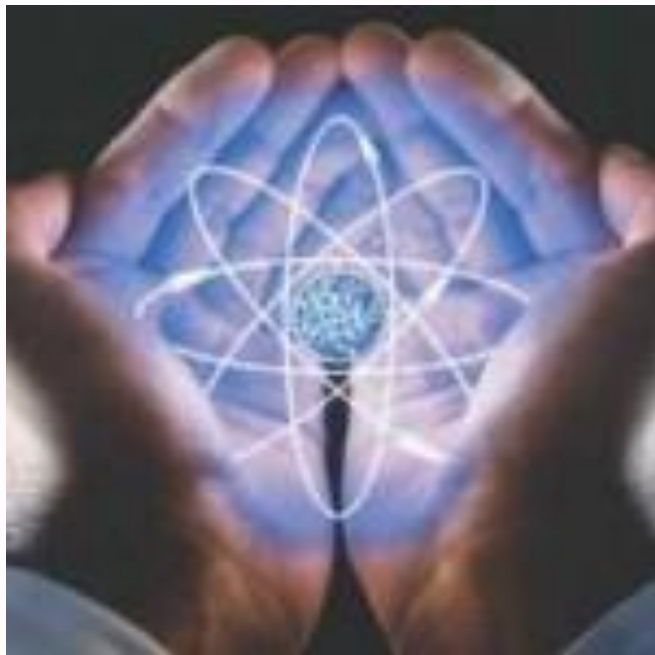
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# El Atomo de Hidrógeno (2)



## Estudio de la Parte Angular

$$\Psi_{n l m}(r, \theta, \varphi) = R_{n l}(r) \cdot \Theta_{l m}(\theta) \cdot \Phi_m(\varphi)$$

$$\Theta_{l m}(\theta) \cdot \Phi_m(\varphi) = Y_m = \text{Armónicos esféricos}$$

$m = 0$        $Y_m$  función real      Solución matemática = Orbital Atómico

$m \neq 0$        $Y_m$  función imaginaria ( $i = \sqrt{-1}$ )      Solución matemática =  $i$ ?

**Herramienta matemática:** Si dos o más funciones son solución de una determinada ecuación diferencial, cualquier combinación lineal de ellas será igualmente solución de la misma ecuación diferencial.

Solución *matemáticamente* válida

Pero de todas las posibles combinaciones lineales, sólo aquellas que sean normales, continuas, uniformes, ... será válidas físicamente, ***soluciones aceptables***.

\* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., "Inorganic Chemistry", 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

## Estudio de la Parte Angular

$$n = 2 \quad l = 1 \quad m = 0 \quad Y_0 = \sqrt{\frac{3}{8\pi}} (z/r)$$

$$p_z = \sqrt{\frac{3}{8\pi}} (z/r)$$

$$n = 2 \quad l = 1 \quad m = \pm 1 \quad Y_{\pm 1} = \sqrt{\frac{3}{8\pi}} [(x \pm iy)/r]$$

$$Y_l^{real} = \frac{1}{\sqrt{2}} [Y_l^m + Y_l^{-m}]$$

$$p_x = \sqrt{\frac{3}{4\pi}} (x/r)$$

$$Y_l^{real} = \frac{1}{\sqrt{2}} [Y_l^m - Y_l^{-m}]$$

$$p_y = \sqrt{\frac{3}{4\pi}} (y/r)$$

\* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., "Inorganic Chemistry", 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

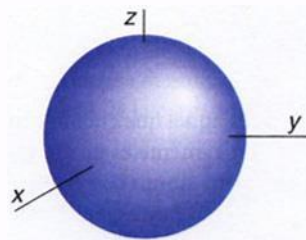
## Estudio de la Parte Angular

Orbital "s"  $\frac{1}{\sqrt{4\pi}}$

Independiente de (x,y,z)  
Sólo depende de "r"

Para cualquier valor "r"  
 $\Theta\Phi$  permanece constante  
 $\Psi$  no varía

$l = 0$     0 nodos angulares    Simetría esférica



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., "Inorganic Chemistry", 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

## Estudio de la Parte Angular

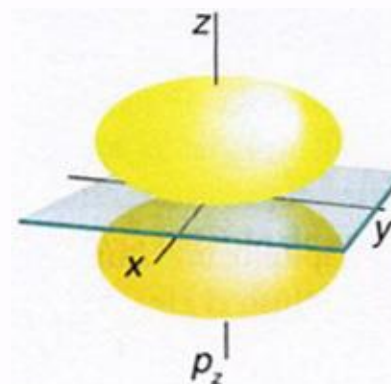
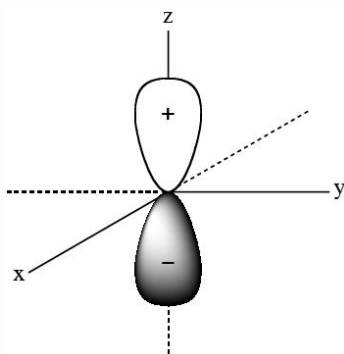
Orbital "p<sub>z</sub>"  $\sqrt{\frac{3}{8\pi}}\left(\frac{z}{r}\right)$  Depende de "z/r"

$l = 1$  1 nodo angular

$z > 0 \quad \Psi > 0 \quad (+)$   
 $z < 0 \quad \Psi < 0 \quad (-)$

$$\sqrt{\frac{3}{8\pi}}\left(\frac{z}{r}\right) = 0 \Rightarrow \left(\frac{z}{r}\right) = 0 \Rightarrow z = 0$$

Plano XY



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4<sup>a</sup> Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., "Inorganic Chemistry", 3<sup>a</sup> Ed., Pearson Prentice Hall, 2008, pp 13.

**Estudio de la Parte Angular**

Orbital “ $p_x$ ”  $\sqrt{\frac{3}{4\pi}}\left(\frac{x}{r}\right)$  Depende de “ $x/r$ ”

Orbital “ $p_y$ ”  $\sqrt{\frac{3}{4\pi}}\left(\frac{y}{r}\right)$  Depende de “ $y/r$ ”

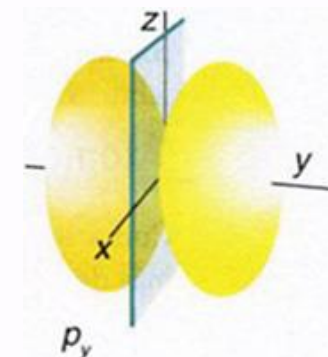
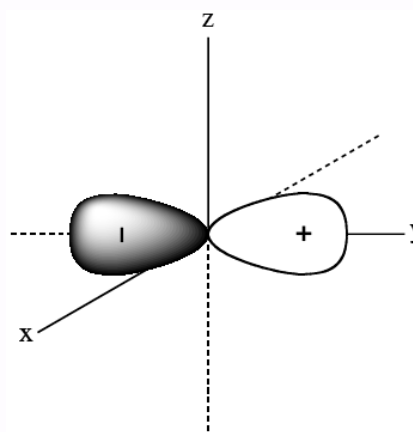
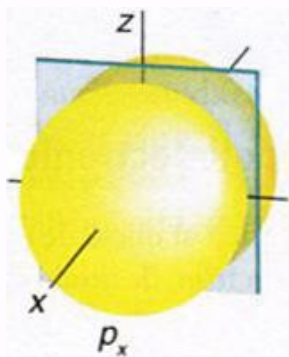
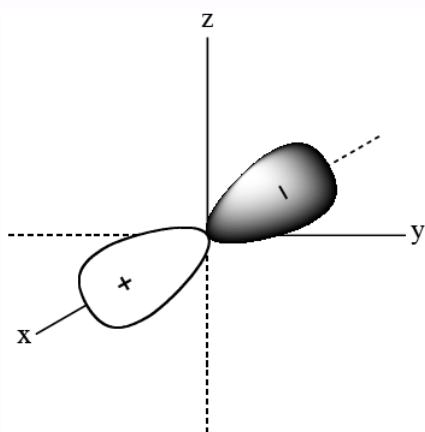
$l = 1$  1 nodo angular

$x > 0$   $\Psi > 0$  (+)  
 $x < 0$   $\Psi < 0$  (-)

$x = 0$   
Plano YZ

$y > 0$   $\Psi > 0$  (+)  
 $y < 0$   $\Psi < 0$  (-)

$y = 0$   
Plano XZ



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., “*Inorganic Chemistry: Principles of Structure and Reactivity*”, 4ª Ed., Harper Collins, 1993, **pp 11**.

\* Moeller, T., “*Inorganic Chemistry. A Modern Introduction*”, John Wiley & Sons, 1994. Traducción española: “*Química Inorgánica*”, Reverté, 1994, **pp 45**.

\* Housecroft, C. E.; Sharpe, A. G., “*Inorganic Chemistry*”, 3ª Ed., Pearson Prentice Hall, 2008, **pp 13**.

## Estudio de la Parte Angular

Orbital “ $d_{z^2}$ ”  $\sqrt{\frac{5}{16\pi}} \{2z^2 - (x^2 + y^2)\} / r^2$

Depende de “ $2z^2 - (x^2 + y^2)$ ”

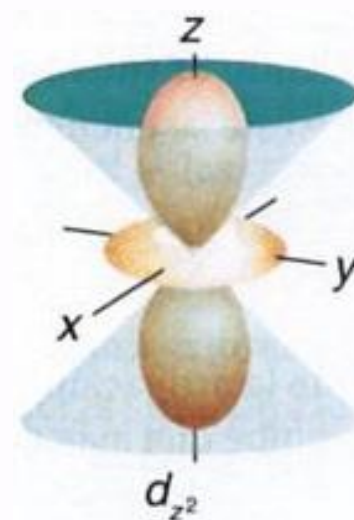
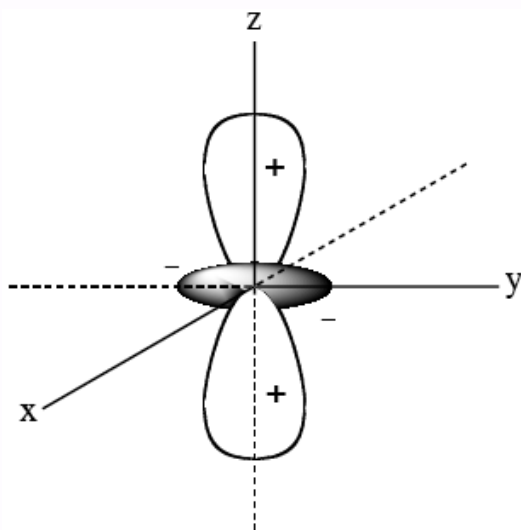
$$\begin{aligned} z > 0 & \quad \Psi > 0 \quad (+) \\ z < 0 & \quad \Psi > 0 \quad (+) \\ z = 0 & \quad \Psi < 0 \quad (-) \end{aligned}$$

$l = 2$     2 nodos angulares

$$\{2z^2 - (x^2 + y^2)\} / r^2 = 0 \Rightarrow 2z^2 - (x^2 + y^2) = 0$$

$$2z^2 = x^2 + y^2$$

Circunferencia  
de radio  $\pm z\sqrt{2}$



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., “*Inorganic Chemistry: Principles of Structure and Reactivity*”, 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., “*Inorganic Chemistry. A Modern Introduction*”, John Wiley & Sons, 1994. Traducción española: “*Química Inorgánica*”, Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., “*Inorganic Chemistry*”, 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

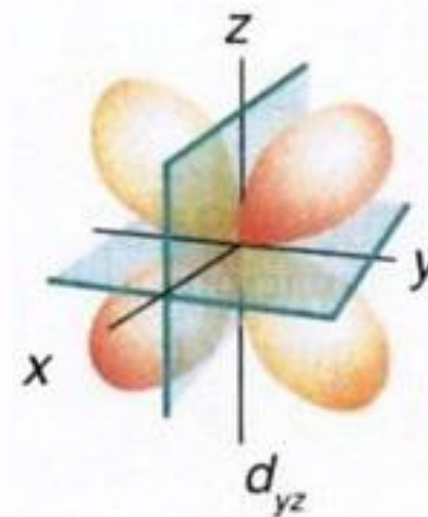
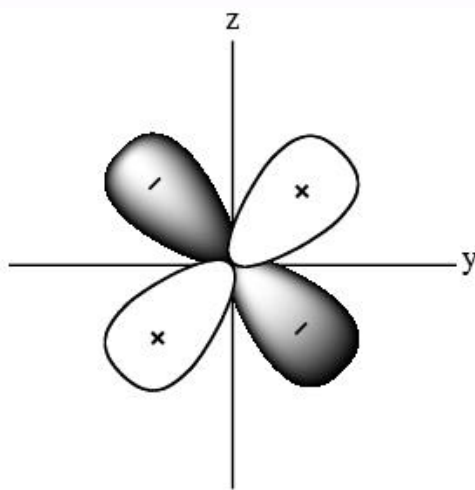
## Estudio de la Parte Angular

Orbital “ $d_{yz}$ ”  $\sqrt{\frac{60}{16\pi}} \frac{yz}{r^2}$  Depende de “ $yz$ ”

$$\begin{aligned} ++ / -- & \Psi > 0 (+) \\ +- / -+ & \Psi < 0 (-) \end{aligned}$$

$l = 2$  2 nodos angulares

$$yz = 0 \begin{cases} y = 0 \text{ plano XZ} \\ z = 0 \text{ plano XY} \end{cases}$$



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., “*Inorganic Chemistry: Principles of Structure and Reactivity*”, 4ª Ed., Harper Collins, 1993, **pp 11**.

\* Moeller, T., “*Inorganic Chemistry. A Modern Introduction*”, John Wiley & Sons, 1994. Traducción española: “*Química Inorgánica*”, Reverté, 1994, **pp 45**.

\* Housecroft, C. E.; Sharpe, A. G., “*Inorganic Chemistry*”, 3ª Ed., Pearson Prentice Hall, 2008, **pp 13**.



**Estudio de la Parte Angular**

Orbital “ $d_{xy}$ ”  $\sqrt{\frac{60}{16\pi}} \frac{xy}{r^2}$  Depende de “xy”

Orbital “ $d_{xz}$ ”  $\sqrt{\frac{60}{16\pi}} \frac{xz}{r^2}$  Depende de “xz”

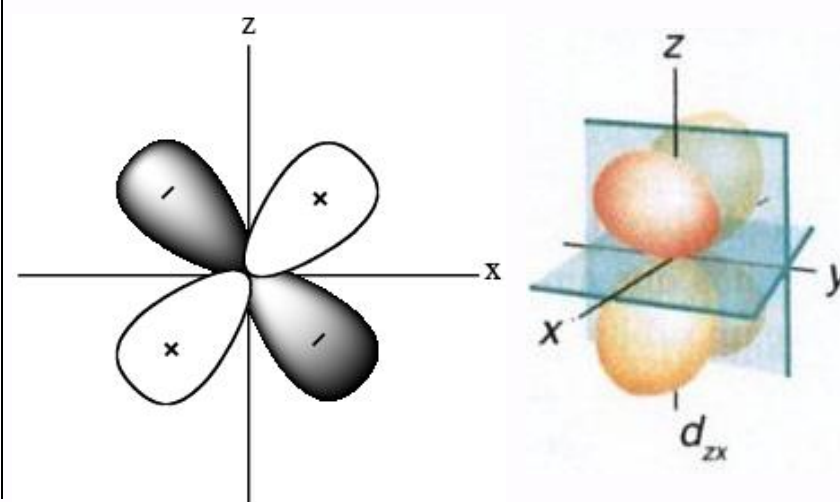
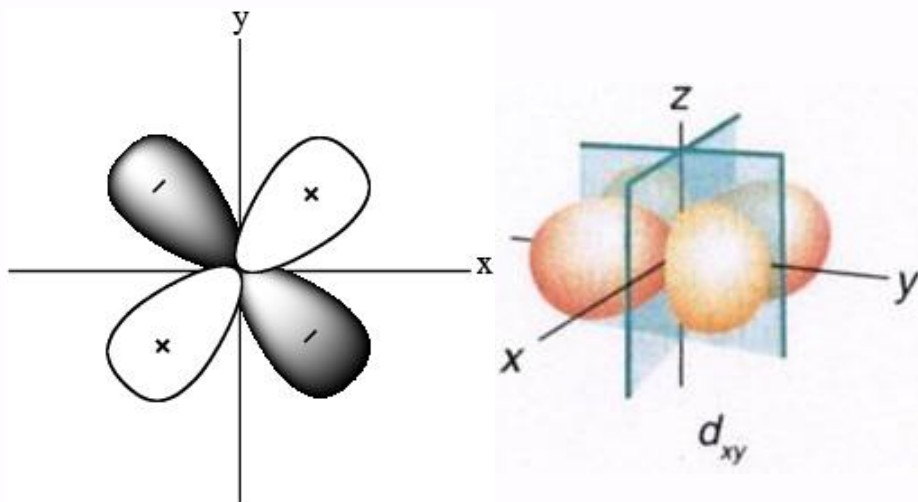
$l = 2$  2 nodos angulares

$++/-- \quad \Psi > 0 (+)$   
 $+--/-+ \quad \Psi < 0 (-)$

$xy = 0 \begin{cases} x = 0 \text{ plano YZ} \\ y = 0 \text{ plano XZ} \end{cases}$

$++/-- \quad \Psi > 0 (+)$   
 $+--/-+ \quad \Psi < 0 (-)$

$xz = 0 \begin{cases} x = 0 \text{ plano YZ} \\ z = 0 \text{ plano XY} \end{cases}$



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., “*Inorganic Chemistry: Principles of Structure and Reactivity*”, 4ª Ed., Harper Collins, 1993, **pp 11**.

\* Moeller, T., “*Inorganic Chemistry. A Modern Introduction*”, John Wiley & Sons, 1994. Traducción española: “*Química Inorgánica*”, Reverté, 1994, **pp 45**.

\* Housecroft, C. E.; Sharpe, A. G., “*Inorganic Chemistry*”, 3ª Ed., Pearson Prentice Hall, 2008, **pp 13**.

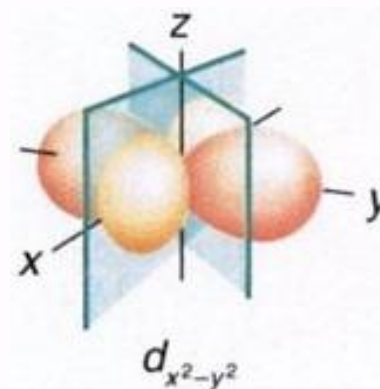
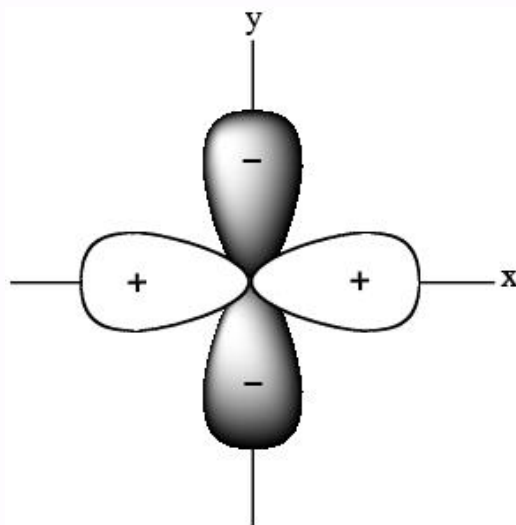
## Estudio de la Parte Angular

Orbital “ $d_{x^2-y^2}$ ”  $\sqrt{\frac{15}{16\pi}} \frac{x^2-y^2}{r^2}$  Depende de “ $x^2-y^2$ ”

$$\begin{aligned} y = 0 & \quad \Psi > 0 \quad (+) \\ x = 0 & \quad \Psi < 0 \quad (-) \end{aligned}$$

$$l = 2 \quad 2 \text{ nodos angulares}$$

$$x^2 - y^2 = 0 \quad \begin{cases} x = +y \text{ plano bisector} \\ x = -y \text{ plano bisector} \end{cases}$$



\* Huheey, J. E., Keiter, R. L., Keiter, E. A., “*Inorganic Chemistry: Principles of Structure and Reactivity*”, 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., “*Inorganic Chemistry. A Modern Introduction*”, John Wiley & Sons, 1994. Traducción española: “*Química Inorgánica*”, Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., “*Inorganic Chemistry*”, 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

## Estudio de la Parte Angular

El signo de  $\Theta(\theta)\Phi(\varphi)$  no tiene nada que ver con la posible carga.

$\Theta(\theta)\Phi(\varphi)$  y  $\Theta^2(\theta)\Phi^2(\varphi)$  son únicamente funciones matemáticas, análogas a  $R(r)$  y  $4\pi r^2 R^2(r)$ . Son representaciones que ayudan a visualizar y obtener información sobre la probable distribución de los electrones.

Se puede definir orbital como:  $\Psi$ ,  $\Psi^2$ ,  $R(r)$ ,  $R^2(r)$ ,  $4\pi r^2 R^2(r)$ ,  $\Theta(\theta)\Phi(\varphi)$  y  $\Theta^2(\theta)\Phi^2(\varphi)$  pero teniendo muy claro que cualquiera de ellas no es más que una función matemática, y que sus representaciones ayudan a visualizar la distribución electrónica, pero no representan al átomo.

\* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4ª Ed., Harper Collins, 1993, pp 11.

\* Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 45.

\* Housecroft, C. E.; Sharpe, A. G., "Inorganic Chemistry", 3ª Ed., Pearson Prentice Hall, 2008, pp 13.

## Estudio conjunto

### Representación

Parte Radial de la función  
 $R(r)$

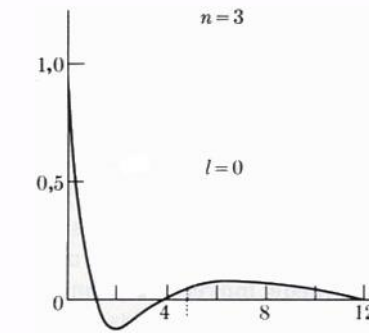
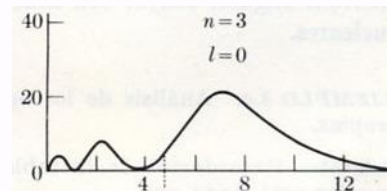


Fig - 4

Función de Distribución Radial  
 $4\pi r^2 R^2(r)$



## Estudio conjunto

### Representación

Parte Angular de la función  
 $\Theta(\theta)\Phi(\varphi)$

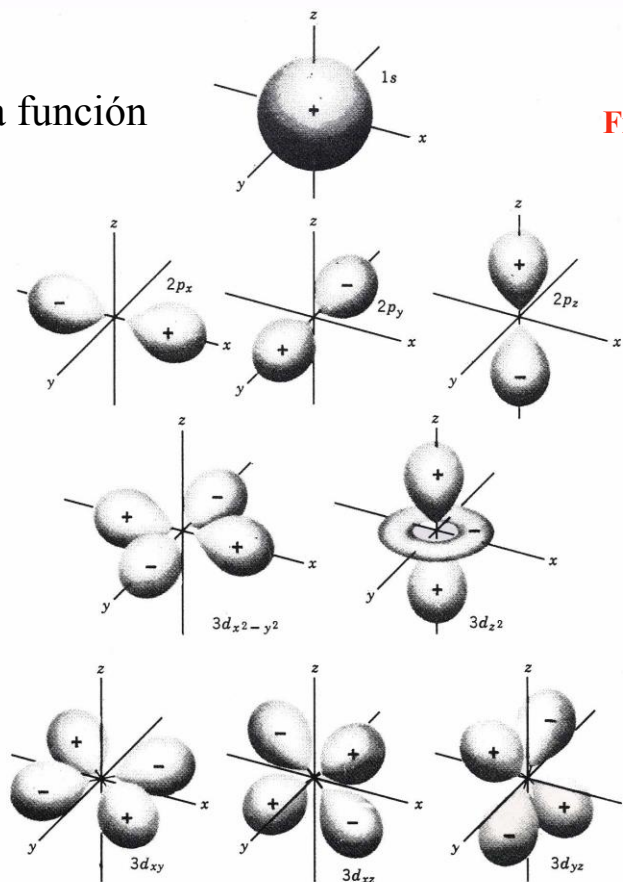


Figura 2-15 Representaciones tridimensionales que muestran la dependencia angular de los orbitales 1s, 2p y 3d para  $r$  fijo. [F. Daniels and R. A. Alberty, *Physical Chemistry*, 4.ª ed., pág. 416, John Wiley et Sons, Inc., New York (1975).]

Fig - 5

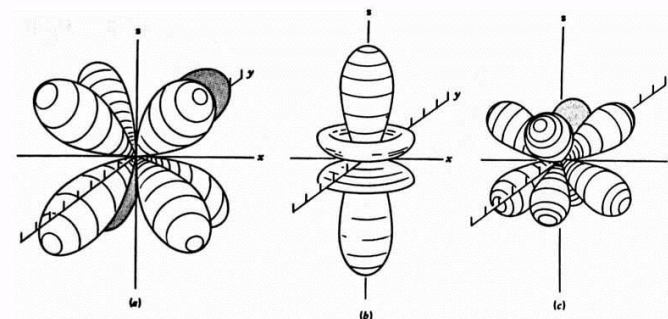


Figure 2-17 Representations of 4f orbitals. (a)  $f_{xyz}$ ; (b)  $f_{z(5z^2-3z^2)}$ ; (c)  $f_{z(x^2-y^2)}$  [J. T. Waber and J. E. Hockett, in *Proceedings of the Fourth Conference on Rare Earth Research*, L. Eyring (Ed.), Fig. 1, p. 285, Gordon and Breach, New York (1965).]

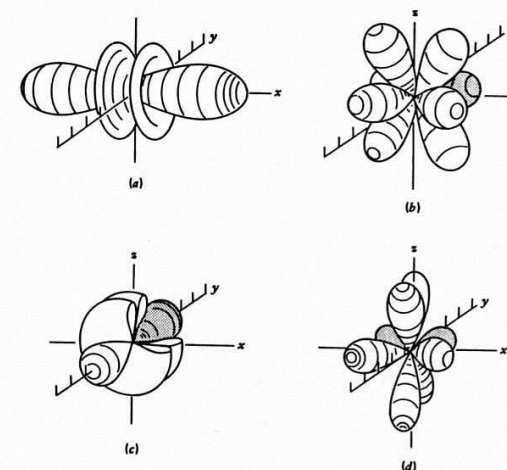


Figure 2-18 Representations of 4f orbitals. (a)  $f_x(5x^2-3x^2)$ ; (b)  $f_x(x^2-y^2)$ ; (c)  $f_y(5y^2-3y^2)$ ; (d)  $f_y(x^2-y^2)$ . [J. T. Waber and J. E. Hockett, in *Proceedings of the Fourth Conference on Rare Earth Research*, L. Eyring (Ed.), Fig. 3, p. 287, Gordon and Breach, New York (1965).]

Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994.

Traducción española: "Química Inorgánica", Reverté, 1994, pp 55 y 57.

## Estudio conjunto

### Representación

Mapas de densidad electrónica 3D

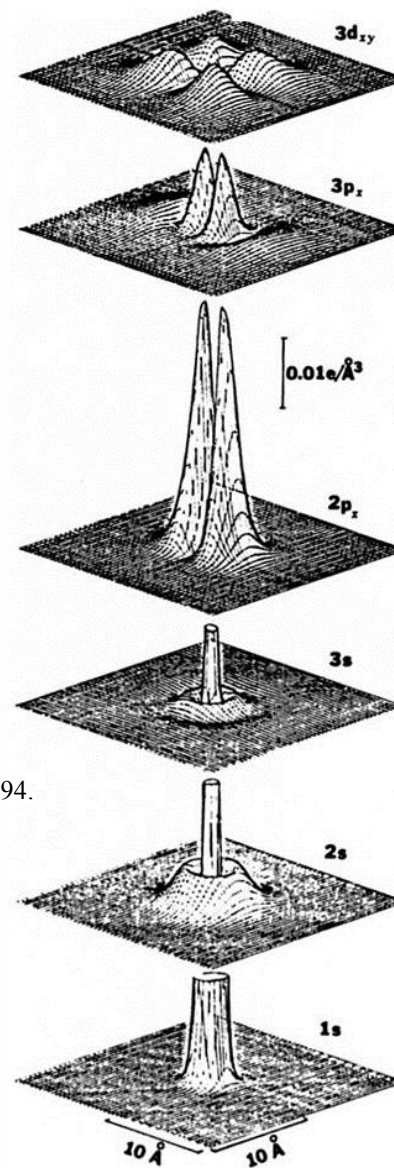


Fig - 6

Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994.  
Traducción española: "Química Inorgánica", Reverté, 1994, pp 56

## Estudio conjunto

### Representación

Diagrama de puntos

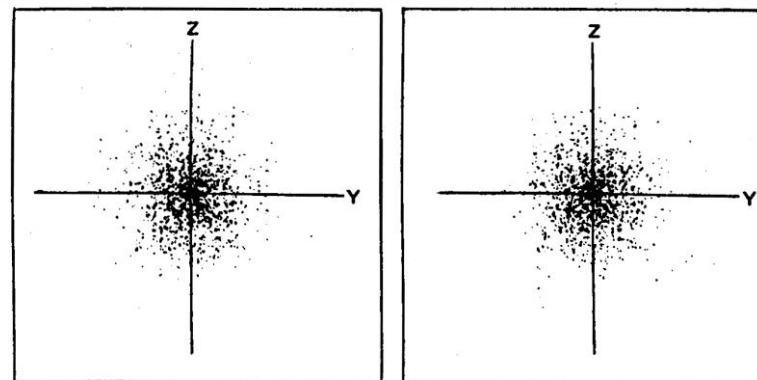


Figure 2-13 Electron-density map for hydrogenic 1s orbital. [D. T. Cromer, *J. Chem. Educ.*, 45, 626 (1968), Fig. 1.]

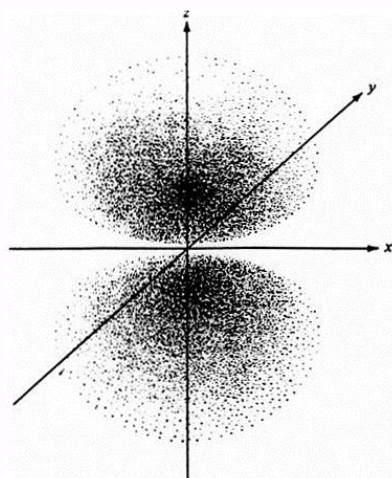


Fig - 7

Moeller, T., "Inorganic Chemistry. A Modern Introduction", John Wiley & Sons, 1994. Traducción española: "Química Inorgánica", Reverté, 1994, pp 53.

Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 4ª Ed., Harper Collins, 1993, pp 16.

Fig. 2.8 Pictorial representation of electron density in a hydrogen-like 2p orbital.