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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 = ¿?

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.

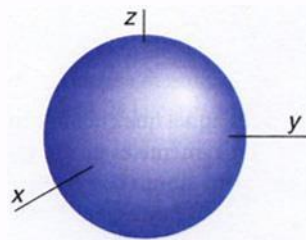
Estudio de la Parte Angular

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

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

Para cualquier valor "r"
 $\Theta\Phi$ permanece constante
 Ψ 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.

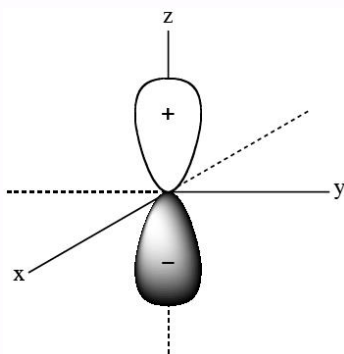
Estudio de la Parte Angular

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

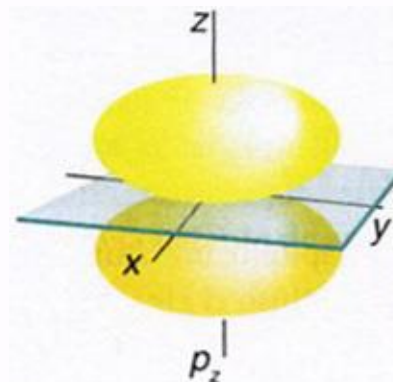
$l = 1$ 1 nodo angular

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

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



Plano XY



* Huheey, J. E., Keiter, R. L., Keiter, E. A., "Inorganic Chemistry: Principles of Structure and Reactivity", 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_x ” $\sqrt{\frac{3}{4\pi}}\left(\frac{x}{r}\right)$

Depende de “ x/r ”

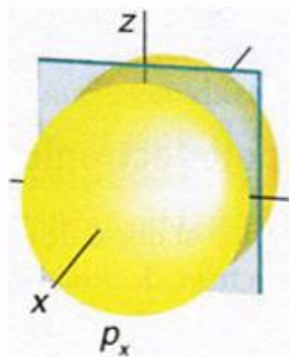
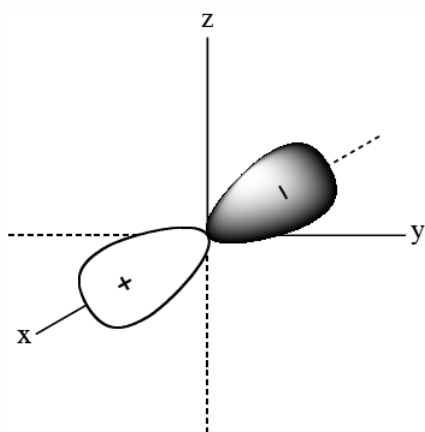
Orbital “ p_y ” $\sqrt{\frac{3}{4\pi}}\left(\frac{y}{r}\right)$

Depende de “ y/r ”

$l = 1$ 1 nodo angular

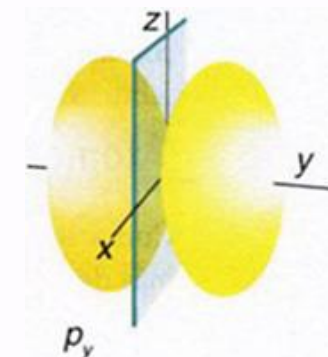
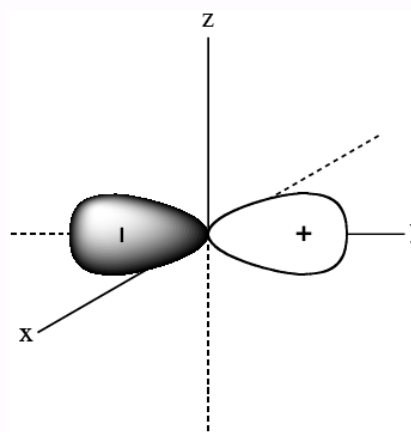
$x > 0$ $\Psi > 0$ (+)
 $x < 0$ $\Psi < 0$ (-)

$x = 0$
 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 “ $2z^2 - (x^2 + y^2)$ ”

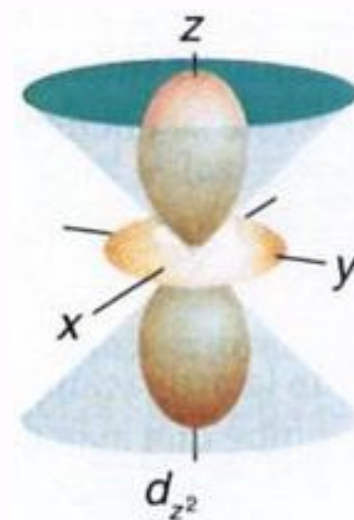
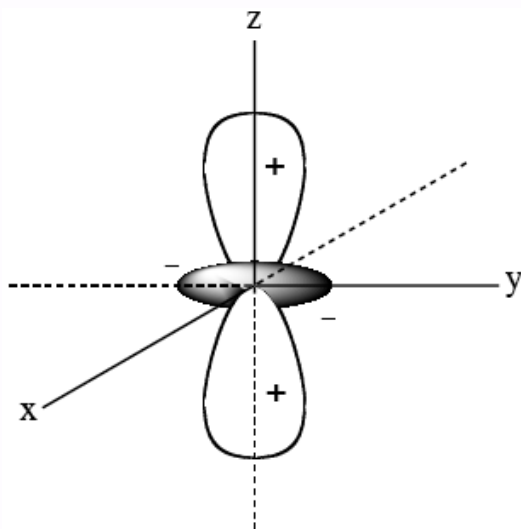
$$\begin{aligned} z > 0 & \quad \Psi > 0 \quad (+) \\ z < 0 & \quad \Psi > 0 \quad (+) \\ z = 0 & \quad \Psi < 0 \quad (-) \end{aligned}$$

$l = 2$ 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.

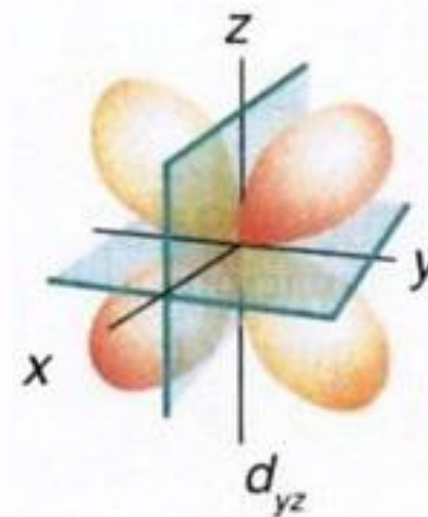
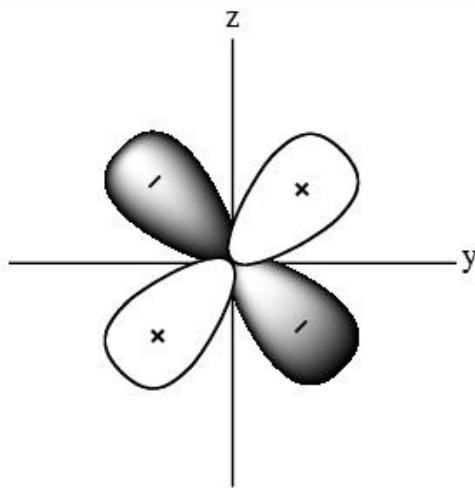
Estudio de la Parte Angular

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”

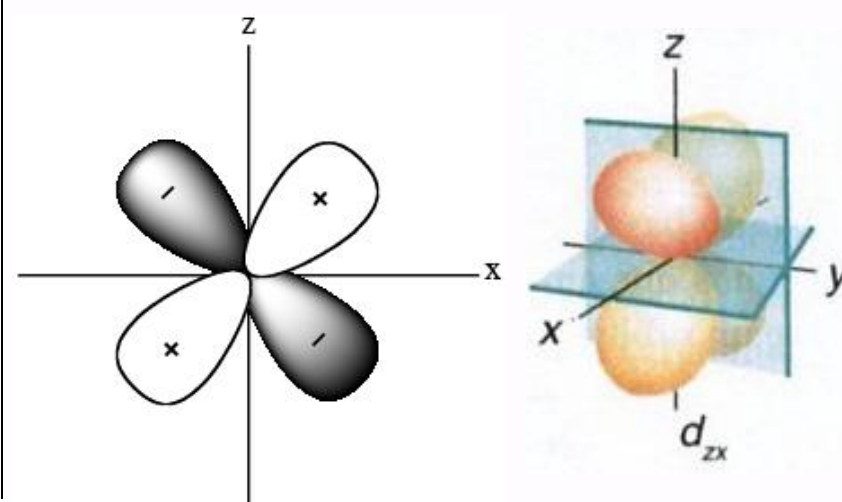
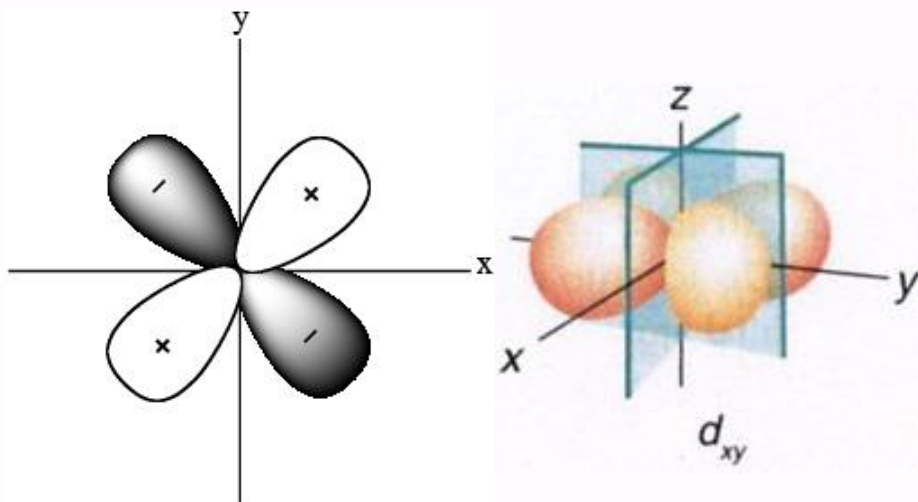
$l = 2$ 2 nodos angulares

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

$xy = 0 \quad \left\{ \begin{array}{l} x = 0 \text{ plano YZ} \\ y = 0 \text{ plano XZ} \end{array} \right.$

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

$xz = 0 \quad \left\{ \begin{array}{l} x = 0 \text{ plano YZ} \\ z = 0 \text{ plano XY} \end{array} \right.$



* 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.

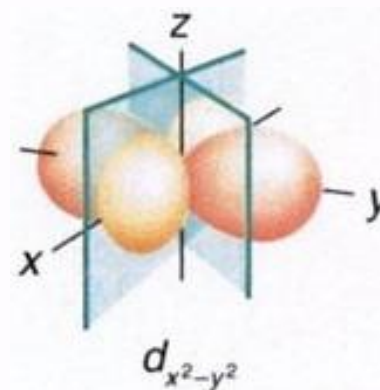
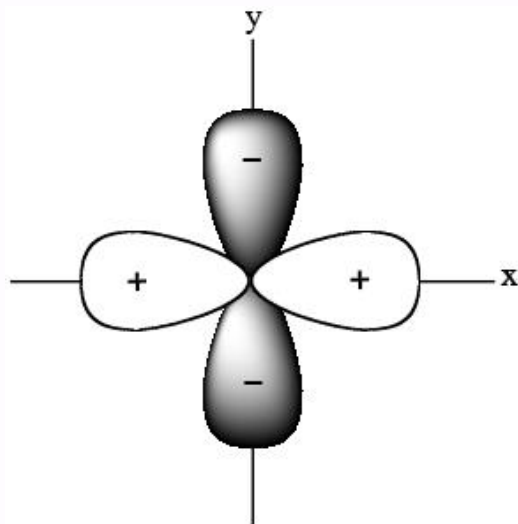
Estudio de la Parte Angular

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: Ψ , Ψ^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
 $R(r)$

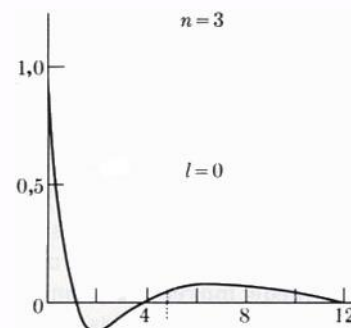
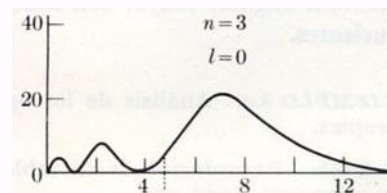


Fig - 4

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



Estudio conjunto

Representación

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

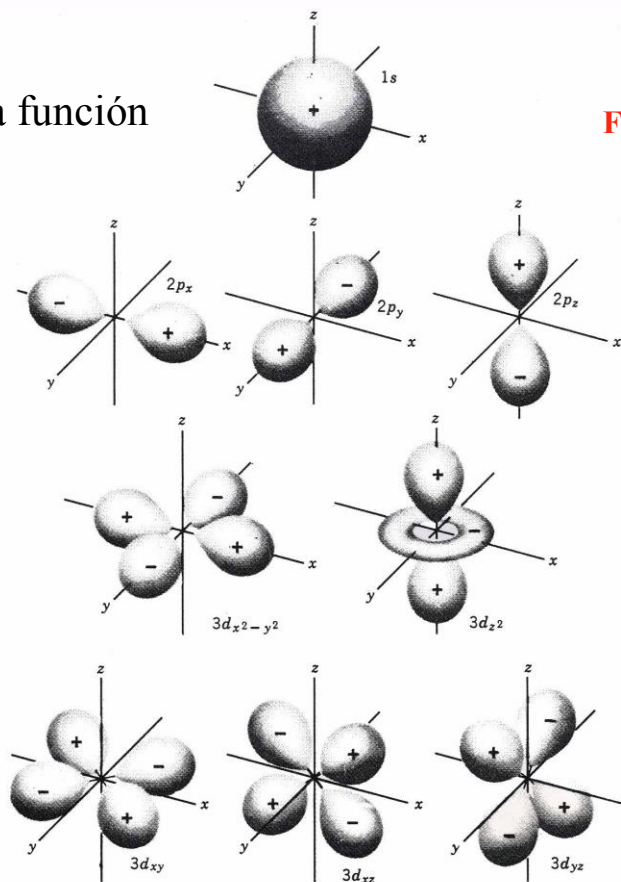


Figura 2-15 Representaciones tridimensionales que muestran la dependencia angular de los orbitales 1s, 2p y 3d para r fijo. [F. Daniels and R. A. Alberty, *Physical Chemistry*, 4.ª ed., pág. 416, John Wiley et Sons, Inc., New York (1975).]

Fig - 5

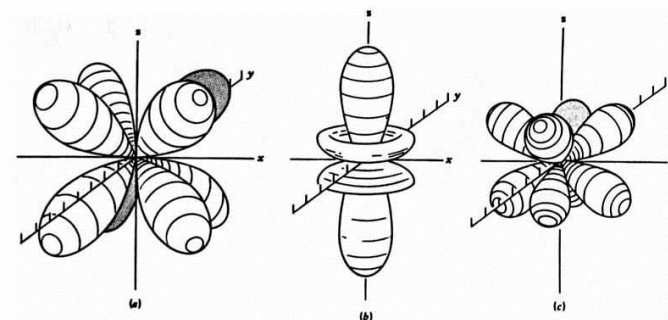


Figure 2-17 Representations of 4f orbitals. (a) f_{x,y,z^2} ; (b) $f_{z(5z^2-3r^2)}$; (c) $f_{z(x^2-y^2)}$ [J. T. Waber and J. E. Hockett, in *Proceedings of the Fourth Conference on Rare Earth Research*, L. Eyring (Ed.), Fig. 1, p. 285, Gordon and Breach, New York (1965).]

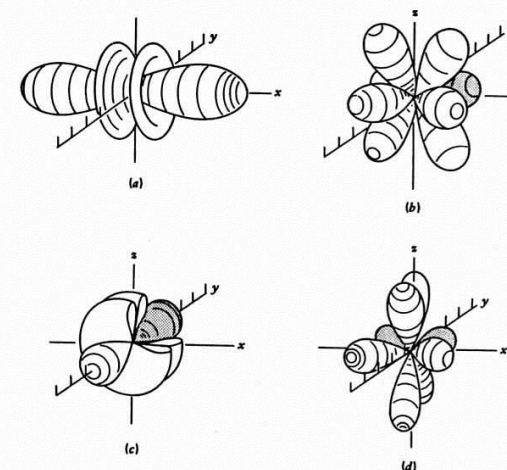


Figure 2-18 Representations of 4f orbitals. (a) $f_{x(5x^2-3r^2)}$; (b) $f_{x(x^2-y^2)}$; (c) $f_{y(5y^2-3r^2)}$; (d) $f_{y(y^2-x^2)}$ [J. T. Waber and J. E. Hockett, in *Proceedings of the Fourth Conference on Rare Earth Research*, L. Eyring (Ed.), Fig. 3, p. 287, Gordon and Breach, New York (1965).]

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

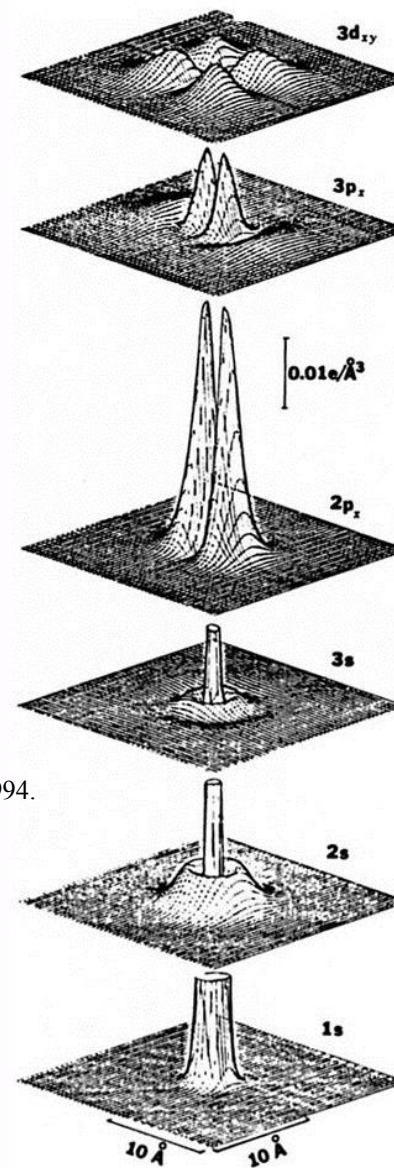


Fig - 6

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

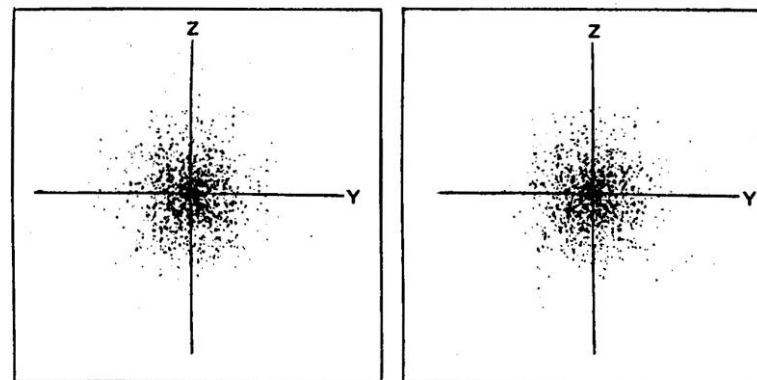


Figure 2-13 Electron-density map for hydrogenic 1s orbital. [D. T. Cromer, *J. Chem. Educ.*, 45, 626 (1968), Fig. 1.]

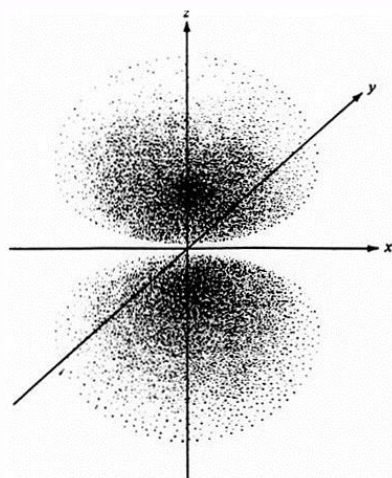


Fig - 7

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", 4^a Ed., Harper Collins, 1993, pp 16.

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