Guía 1, Anexos

En el **Anexo 1** incluimos algunas integrales de utilidad. En el **Anexos 2 y 3** se dan las expresiones de las funciones hidrogénicas, radiales y angulares (armónicos esféricos).

Anexo 1

Integrales útiles:

$$\int_0^\infty r^k\, e^{-z\,r}\, dr = \frac{k!}{z^{k+1}}$$

$$\int d\vec{r}\, \frac{1}{r}\, e^{-zr} e^{i\vec{k}.\vec{r}} = \frac{4\pi}{z^2+k^2}$$

$$\int d\vec{r}\, e^{-zr} e^{i\vec{k}.\vec{r}} = \frac{8\pi\, z}{(z^2+k^2)^2}$$

$$\int d\vec{r}\, r\, e^{-zr} e^{i\vec{k}.\vec{r}} = \frac{8\pi(3z^2-k^2)}{(z^2+k^2)^3}$$

$$\int d\vec{r}\, r^n\, e^{-zr} e^{i\vec{k}.\vec{r}} = -\frac{\partial^n}{\partial z^n}\left(\frac{8\pi\, z}{(z^2+k^2)^2}\right)$$

$$\int d\vec{r}\, r\,(\hat{r}.\hat{e}_j)\, e^{-zr} e^{i\vec{k}.\vec{r}} = -\frac{32\,\pi\, i\;z}{(z^2+k^2)^3}\vec{k}.\hat{e}_j$$

Radios médios:

$$\langle r \rangle_{nlm} = \frac{n^2}{Z}\left\{1+\tfrac{1}{2}\left(1-\frac{l(l+1)}{n^2}\right)\right\}$$

$$\langle 1/r \rangle_{nlm} = \frac{Z}{n^2}$$

$$\langle 1/r^2 \rangle_{nlm} = \frac{Z^2}{n^3}\frac{1}{(l+1/2)}$$

$$\langle 1/r^3 \rangle_{nlm} = \frac{Z^3}{n^3}\frac{1}{l\,(l+1/2)\,(l+1)}, \quad l \neq 0$$

Anexo 2

Tabla 1. Funciones de onda hidrogénicas

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

$$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}\,e^{-Zr/2a_0}\cos\theta$$

$$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}\,e^{-Zr/2a_0}\sin\theta\, e^{\pm i\phi}$$

$$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(27 - 18\,\frac{Zr}{a_0} + 2\,\frac{Z^2r^2}{a_0^2}\right)e^{-Zr/3a_0}$$

$$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6 - \frac{Zr}{a_0}\right)\frac{Zr}{a_0}\,e^{-Zr/3a_0}\cos\theta$$

$$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6 - \frac{Zr}{a_0}\right)\frac{Zr}{a_0}\,e^{-Zr/3a_0}\sin\theta\, e^{\pm i\phi}$$

$$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}\,e^{-Zr/3a_0}(3\cos^2\theta - 1)$$

$$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}\,e^{-Zr/3a_0}\sin\theta\cos\theta\, e^{\pm i\phi}$$

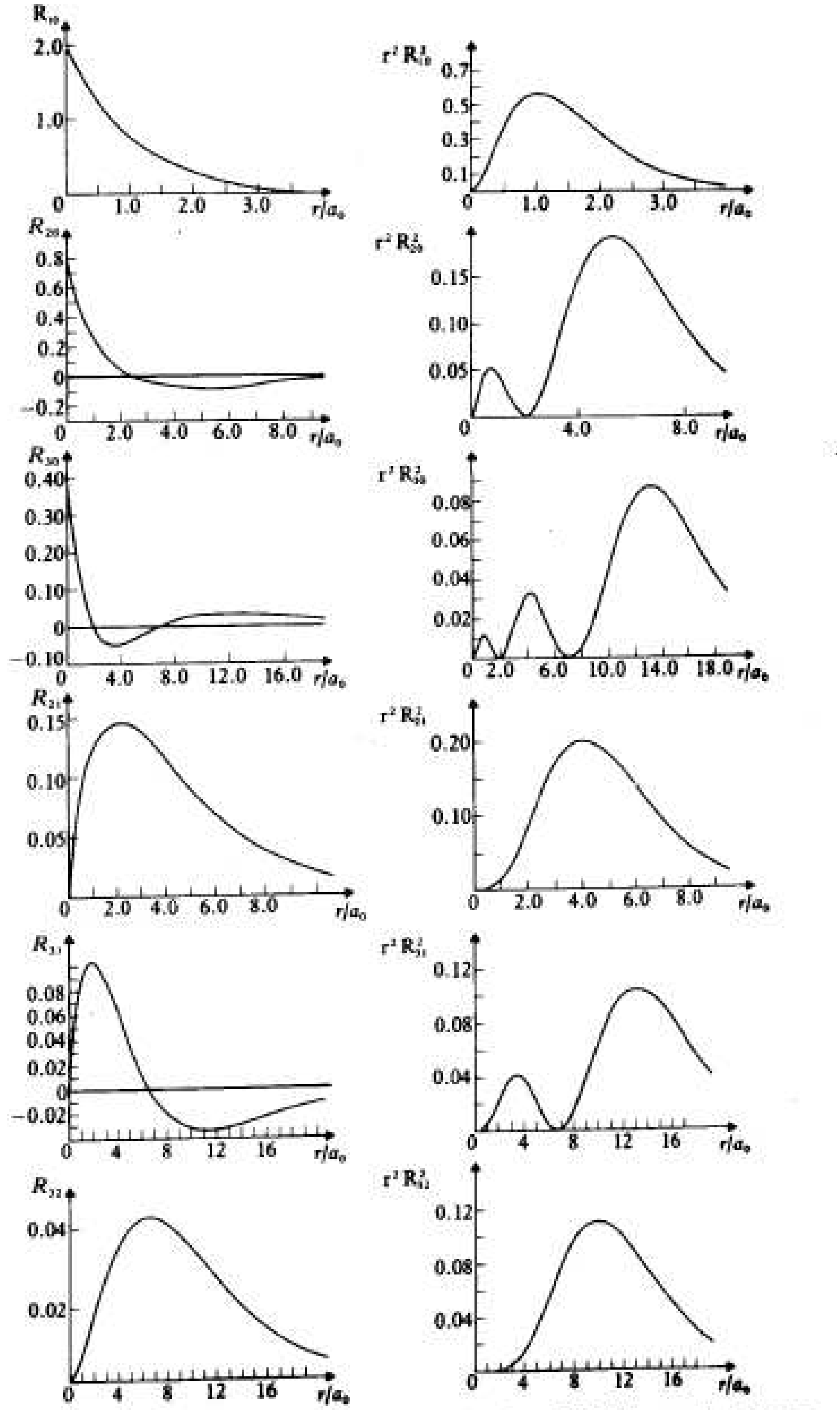
$$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}\,e^{-Zr/3a_0}\sin^2\theta\, e^{\pm 2i\phi}$$

Tabla 2: Funciones de onda radiales R_{nl} de átomos hidrogenoides.

Designación	n	l	$R_{nl}(r)$[a]
$1s$	1	0	$(Z/a_0)^{3/2}\,2\exp(-\rho/2)$
$2s$	2	0	$(Z/a_0)^{3/2}\,8^{-1/2}(2-\rho)\exp(-\rho/2)$
$2p$	2	1	$(Z/a_0)^{3/2}\,24^{-1/2}\rho\exp(-\rho/2)$
$3s$	3	0	$(Z/a_0)^{3/2}\,243^{-1/2}(6-6\rho+\rho^2)\exp(-\rho/2)$
$3p$	3	1	$(Z/a_0)^{3/2}\,486^{-1/2}(4-\rho)\rho\exp(-\rho/2)$
$3d$	3	2	$(Z/a_0)^{3/2}\,2430^{-1/2}\rho^2\exp(-\rho/2)$
$4s$	4	0	$(Z/a_0)^{3/2}\,96^{-1}(24-36\rho+12\rho^2-\rho^3)\exp(-\rho/2)$
$4p$	4	1	$(Z/a_0)^{3/2}\,15360^{-1/2}(20-10\rho+\rho^2)\rho\exp(-\rho/2)$
$4d$	4	2	$(Z/a_0)^{3/2}\,46080^{-1/2}(6-\rho)\rho^2\exp(-\rho/2)$
$4f$	4	3	$(Z/a_0)^{3/2}\,322560^{-1/2}\rho^3\exp(-\rho/2)$

[a] $\rho = 2Zr/(na_0)$.

<u>Gráficos de algunas $R_{nl}(r)$</u> (fuente: Bransden y Joachain, Physics of atoms and molecules)



3.3 Radial functions $R_{nl}(r)$ and radial distribution functions $r^2R^2_{nl}(r)$ for atomic hydrogen.

The Spherical Harmonics

$Y_\ell^{m_\ell}(\theta, \phi)$

$$Y_0^0 = \frac{1}{2\sqrt{\pi}}$$

$$Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cdot \cos\,\theta$$

$$Y_1^{\pm 1} = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\cdot \sin\,\theta\cdot e^{\pm i\phi}$$

$$Y_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}}\cdot (3\,\cos^2\,\theta - 1)$$

$$Y_2^{\pm 1} = \mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\cdot \sin\,\theta\cdot \cos\,\theta\cdot e^{\pm i\phi}$$

$$Y_2^{\pm 2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\cdot \sin^2\,\theta\cdot e^{\pm 2i\phi}$$

$$Y_3^0 = \frac{1}{4}\sqrt{\frac{7}{\pi}}\cdot (5\,\cos^3\,\theta - 3\,\cos\,\theta)$$

$$Y_3^{\pm 1} = \mp\frac{1}{8}\sqrt{\frac{21}{\pi}}\cdot \sin\,\theta\cdot (5\,\cos^2\,\theta - 1)\cdot e^{\pm i\phi}$$

$$Y_3^{\pm 2} = \frac{1}{4}\sqrt{\frac{105}{2\pi}}\cdot \sin^2\,\theta\cdot \cos\,\theta\cdot e^{\pm 2i\phi}$$

$$Y_3^{\pm 3} = \mp\frac{1}{8}\sqrt{\frac{35}{\pi}}\cdot \sin^3\,\theta\cdot e^{\pm 3i\phi}$$

Armóninos esféricos

http://www.uniovi.es/~quimica.fisica/qcg/harmonics/charmonics.html