

Tabla 1.1. Las partículas subatómicas

Nombre	Símbolo	Masa	Carga	Descubrimiento
protón	p	$1,673 \cdot 10^{-27}$ kg	$+1,602 \cdot 10^{-19}$ C	Goldstein, 1886
electrón	e	$9,109 \cdot 10^{-31}$ kg	$-1,602 \cdot 10^{-19}$ C	Thomson, 1897
neutrón	n	$1,675 \cdot 10^{-27}$ kg		Chadwick, 1932

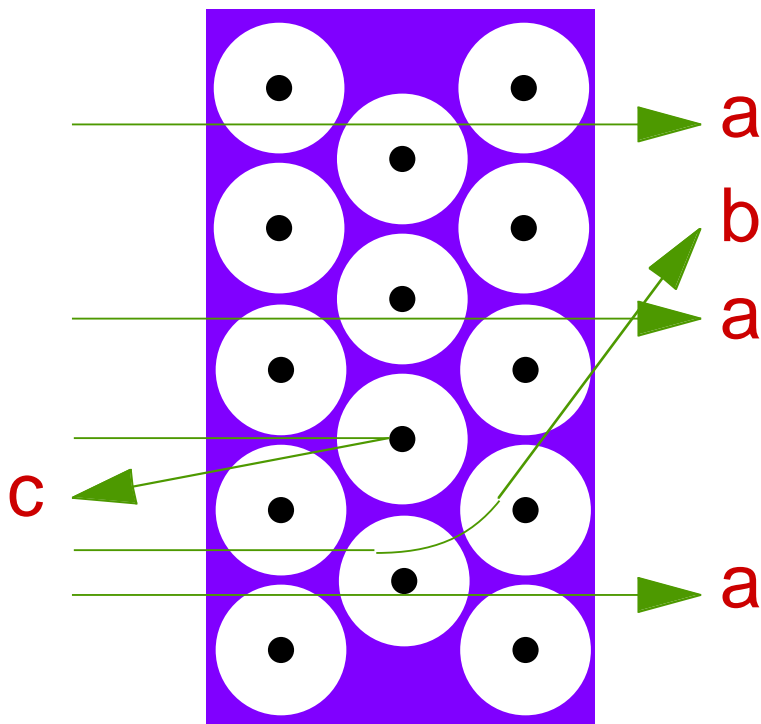
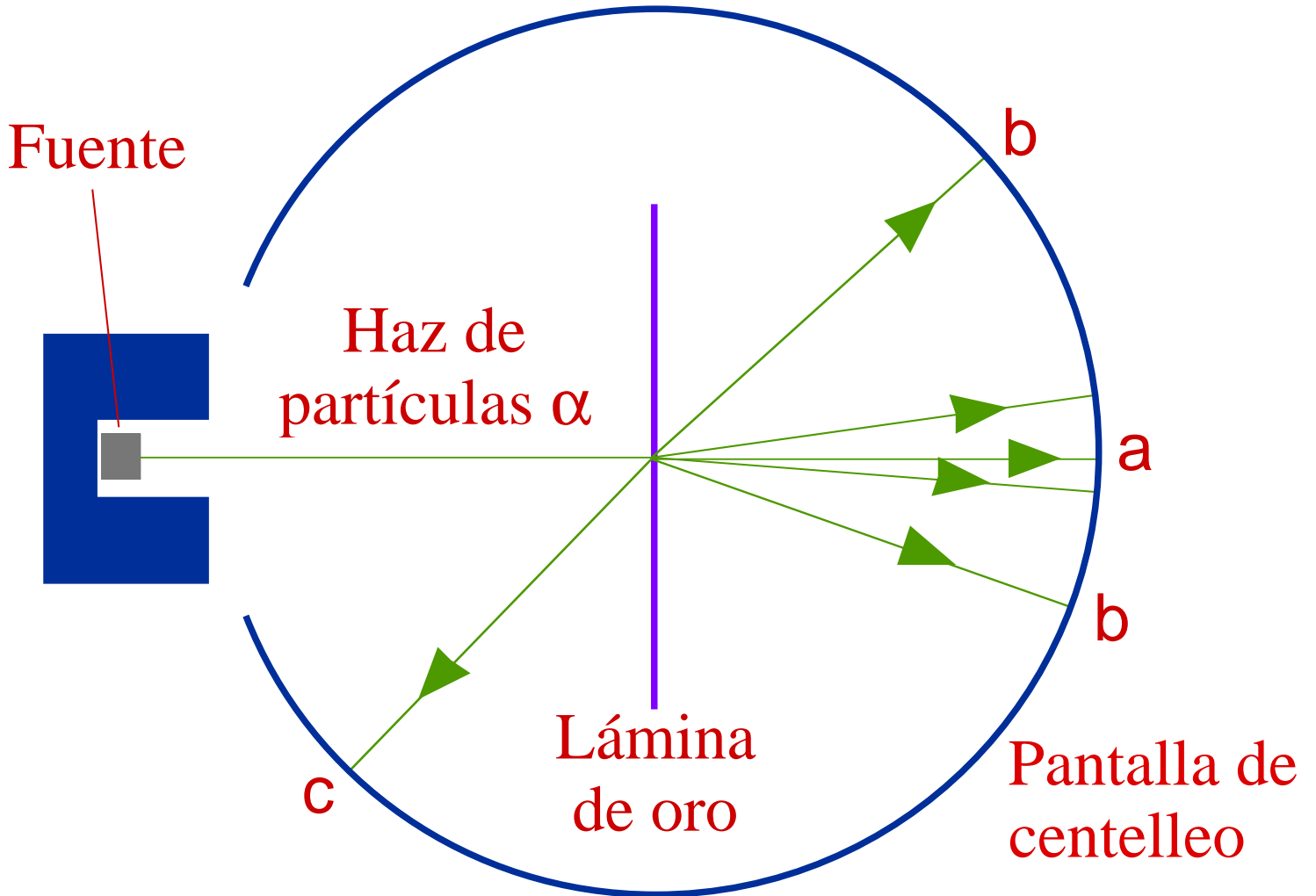
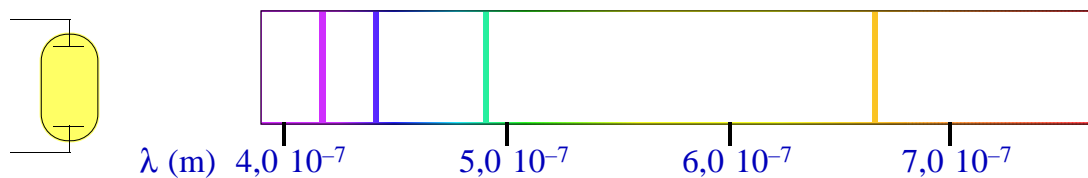
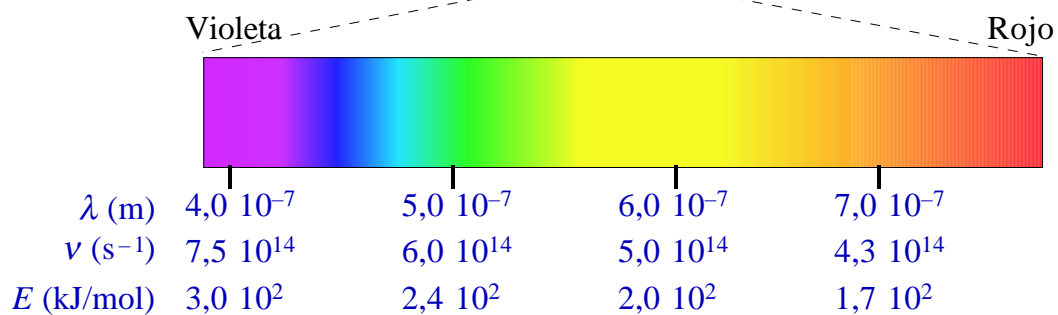
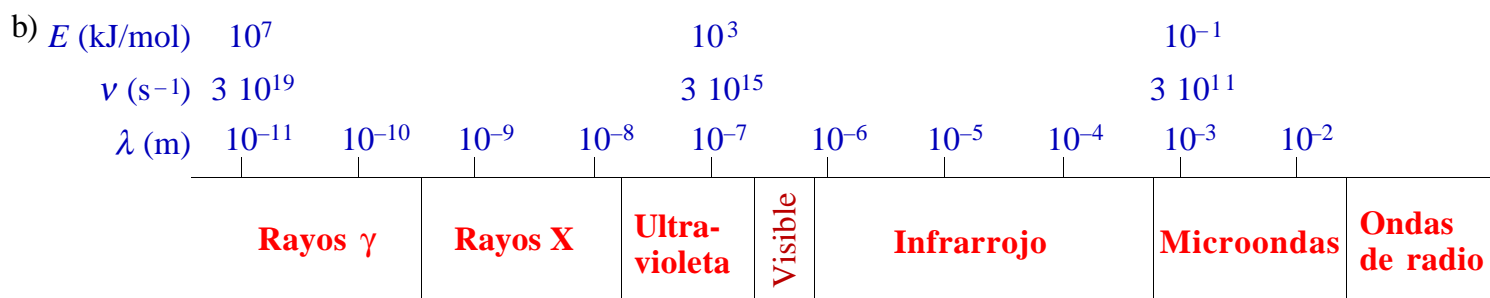
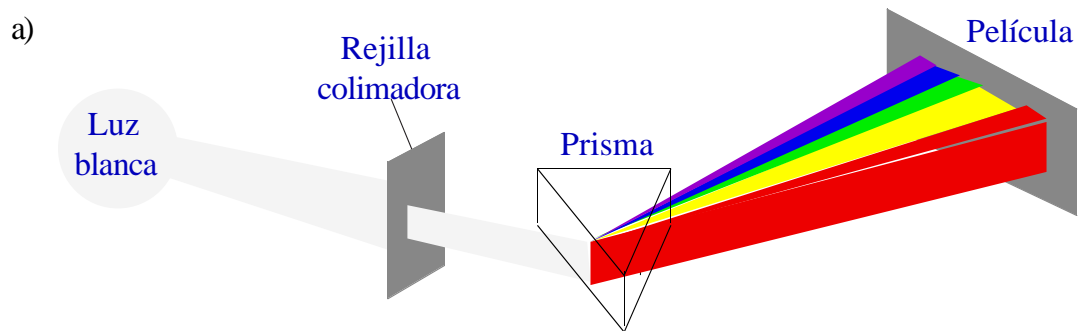
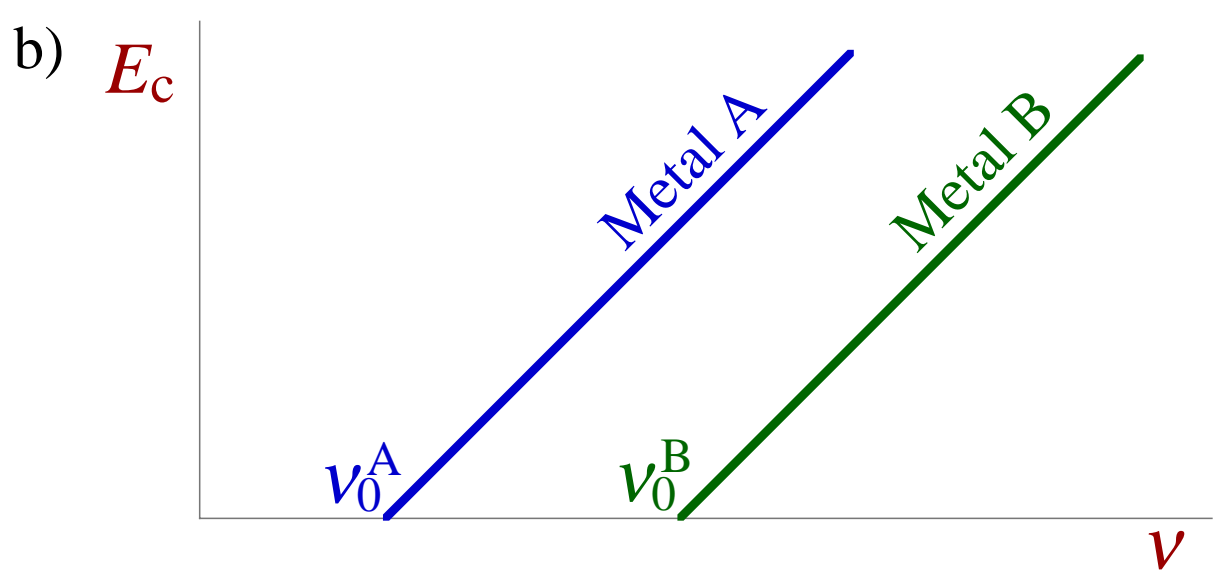
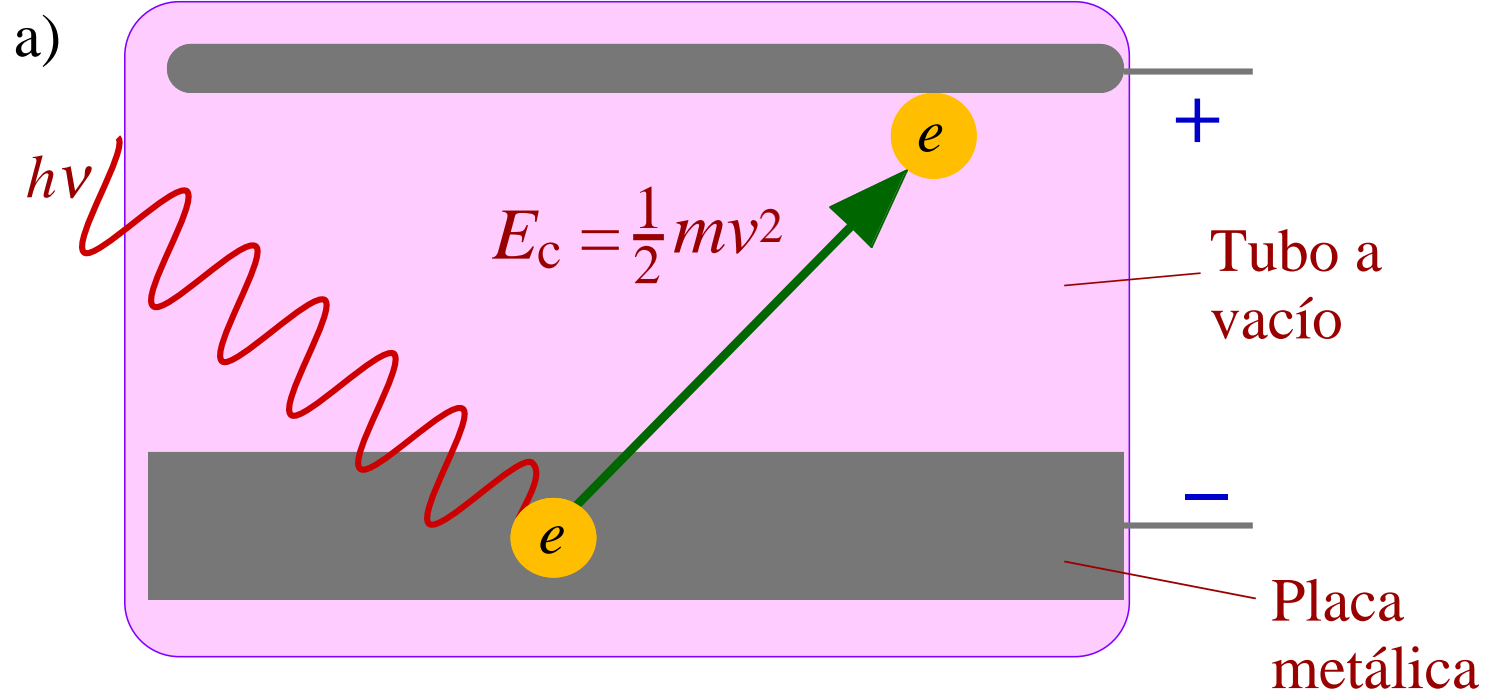
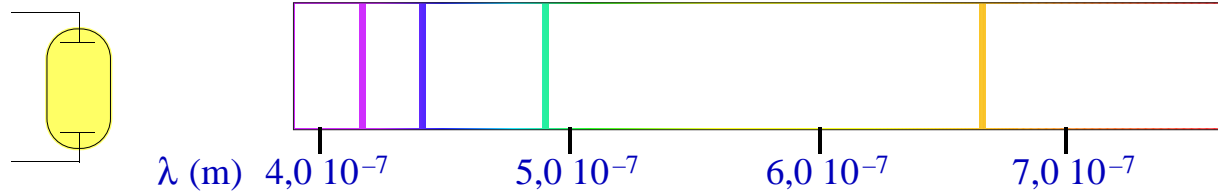


Tabla 1.2. Algunos elementos con varios isótopos

<i>Nombre</i>	<i>Símbolo</i>	<i>Número atómico (Z)</i>	<i>Número neutrónico (N)</i>	<i>Número másico (A)</i>	<i>Masa</i>	<i>Abundancia natural, %</i>
Hidrógeno-1	${}^1\text{H}$	1	0	1	$1,674 \cdot 10^{-24}$ g, 1,008 u	99,985
Deuterio	${}^2\text{H}$ o D	1	1	2	$3,344 \cdot 10^{-24}$ g, 2,014 u	0,015
Tritio	${}^3\text{H}$ o T	1	2	3	$1,674 \cdot 10^{-24}$ g, 3,016 u	muy inestable
Carbono-12	${}^{12}\text{C}$	6	6	12	$1,9926 \cdot 10^{-23}$ g, 12 u exactas	98,90
Carbono-13	${}^{13}\text{C}$	6	7	13	$2,159 \cdot 10^{-23}$ g, 13,00 u	1,10
Cloro-35	${}^{35}\text{Cl}$	17	18	35	$5,807 \cdot 10^{-23}$ g, 34,97 u	75,77
Cloro-37	${}^{37}\text{Cl}$	17	20	37	$6,138 \cdot 10^{-23}$ g, 36,97 u	24,23
Uranio-235	${}^{235}\text{U}$	92	143	235	$3,902 \cdot 10^{-22}$ g, 235,0 u	0,72
Uranio-238	${}^{238}\text{U}$	92	146	238	$3,953 \cdot 10^{-22}$ g, 238,05 u	99,27



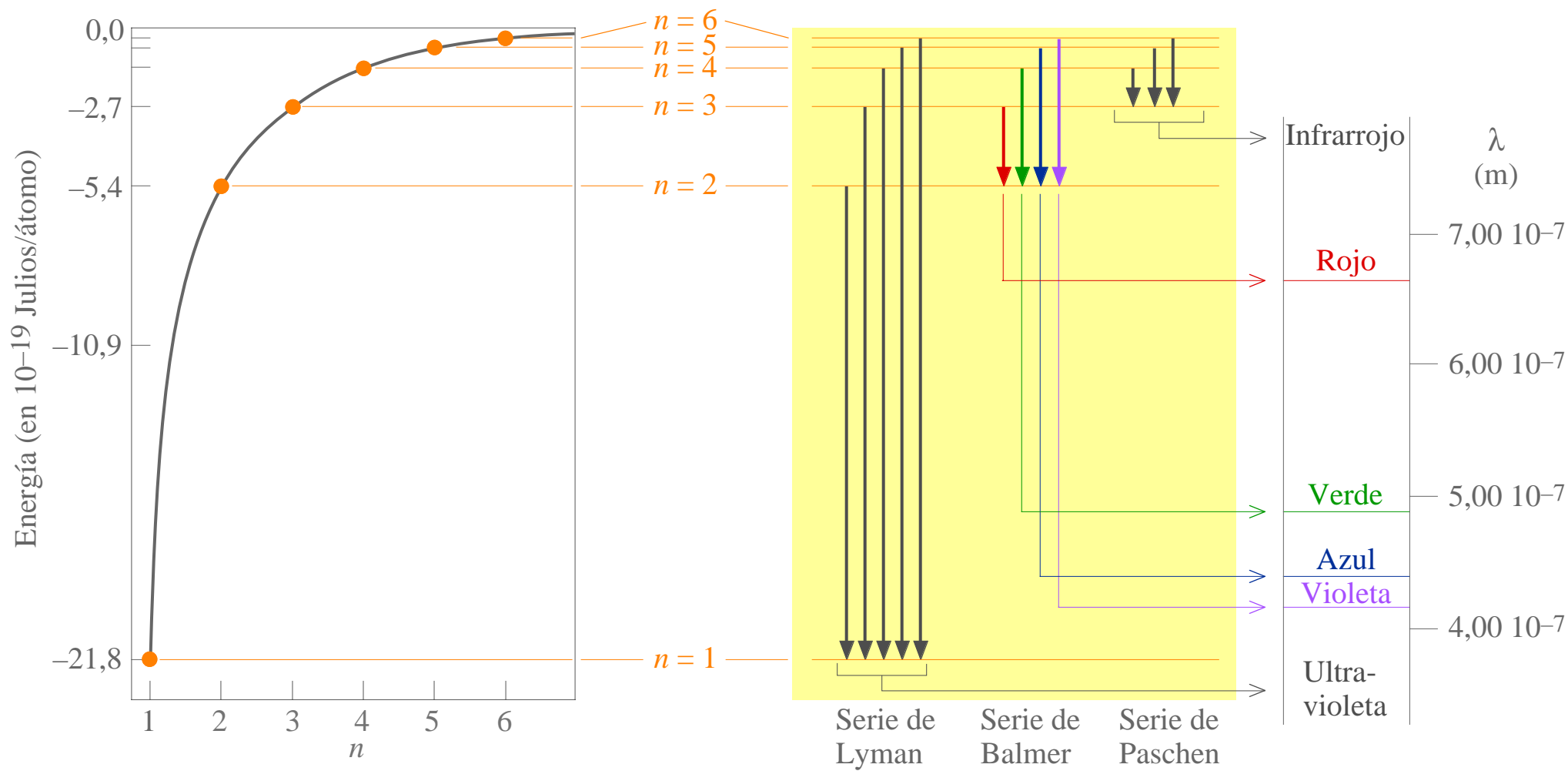




$$\nu = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$R_H = 3,29 \cdot 10^{15} \text{ s}^{-1}$ (constante de Rydberg)

Serie de Lyman	$n_1 = 1$	$n_2 = 2, 3, 4, 5 \dots$	Serie de Brackett	$n_1 = 4$	$n_2 = 5, 6, 7, 8 \dots$
Serie de Balmer	$n_1 = 2$	$n_2 = 3, 4, 5, 6 \dots$	Serie de Pfund	$n_1 = 5$	$n_2 = 6, 7, 8, 9 \dots$
Serie de Pashen	$n_1 = 3$	$n_2 = 4, 5, 6, 7 \dots$			



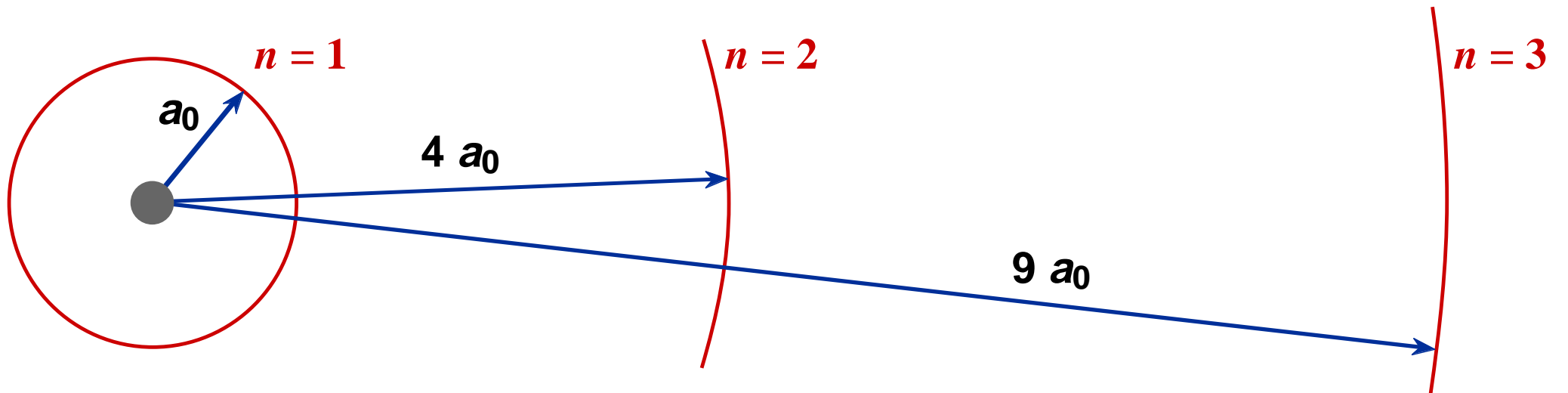


Tabla 1.3. Números cuánticos del átomo de hidrógeno

Nombre	Símbolo	Valores	Nombre de conjunto	Sinónimos	Describe
principal	n	1, 2, 3,...	nivel o capa	K ($n = 1$), L (2), M (3), N (4), etc	tamaño y energía orbital
azimutal*	l	0, ..., $n-1$	subnivel o subcapa	s ($l = 0$), p (1), d (2), f (3), etc	forma del orbital
magnético orbital	m_l	+ l , ..., - l	orbital** de una subcapa		orientación del orbital
de espín	s	$1/2$			espín del electrón
magnético de espín	m_s	$\pm 1/2$			orientación del espín

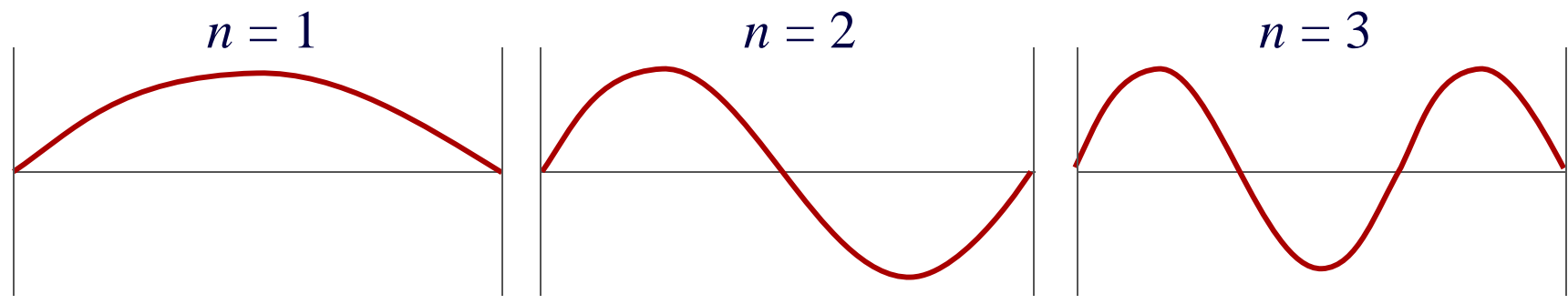
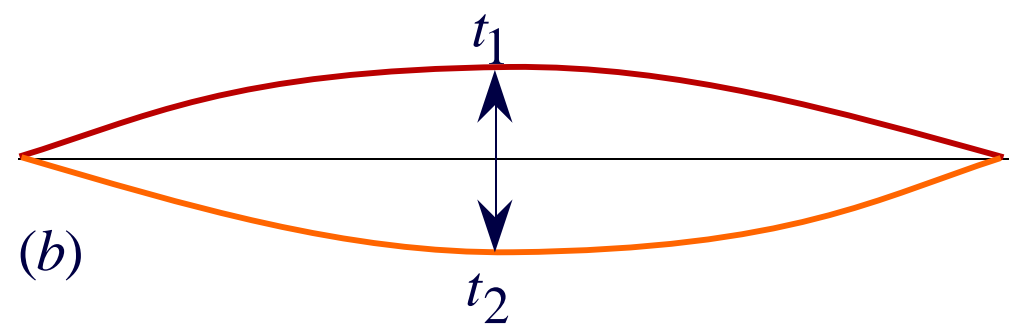
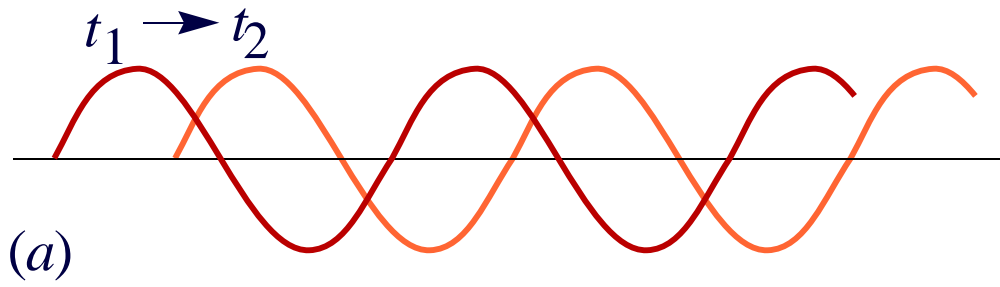
*También llamado momento angular orbital; ***órbita* en el lenguaje de Bohr, *orbital* en el de la mecánica cuántica.

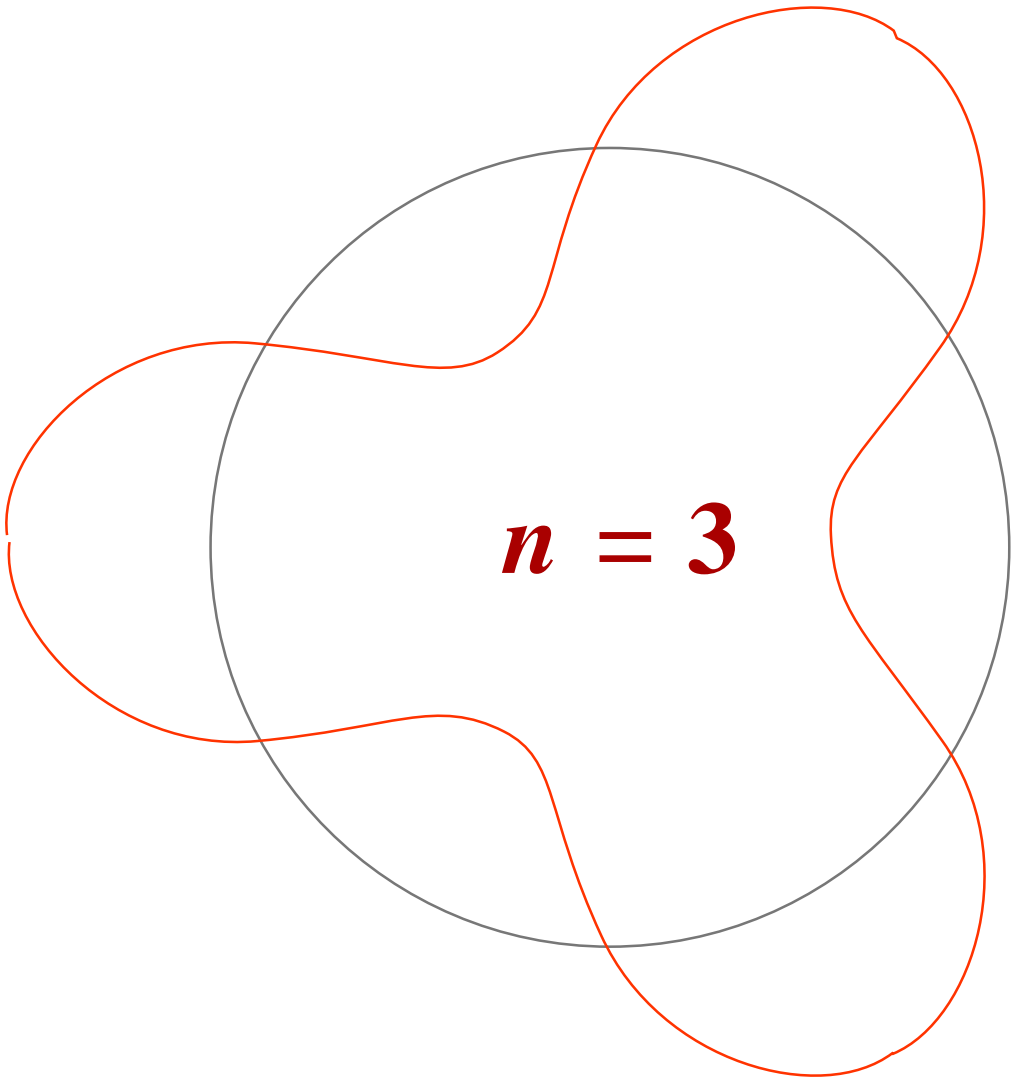
Tabla 1.4. Longitudes de onda de partículas

Partícula	Masa (kg)	Velocidad ($m s^{-1}$)	Longitud de onda (\AA)
Electrón libre gaseoso (300 K)	$9,11 \cdot 10^{-31}$	$1,17 \cdot 10^5$	63
Electrón libre gaseoso ($200 \cdot 10^3$ K)	$9,11 \cdot 10^{-31}$	$3,00 \cdot 10^6$	2,4
Electrón del átomo de H ($n = 1$)	$9,11 \cdot 10^{-31}$	$2,19 \cdot 10^6$	3,3
Átomo de He gaseoso (300 K)	$6,64 \cdot 10^{-27}$	1370	0,73
Pelota de Béisbol	0,10	20	$3,3 \cdot 10^{-24}$

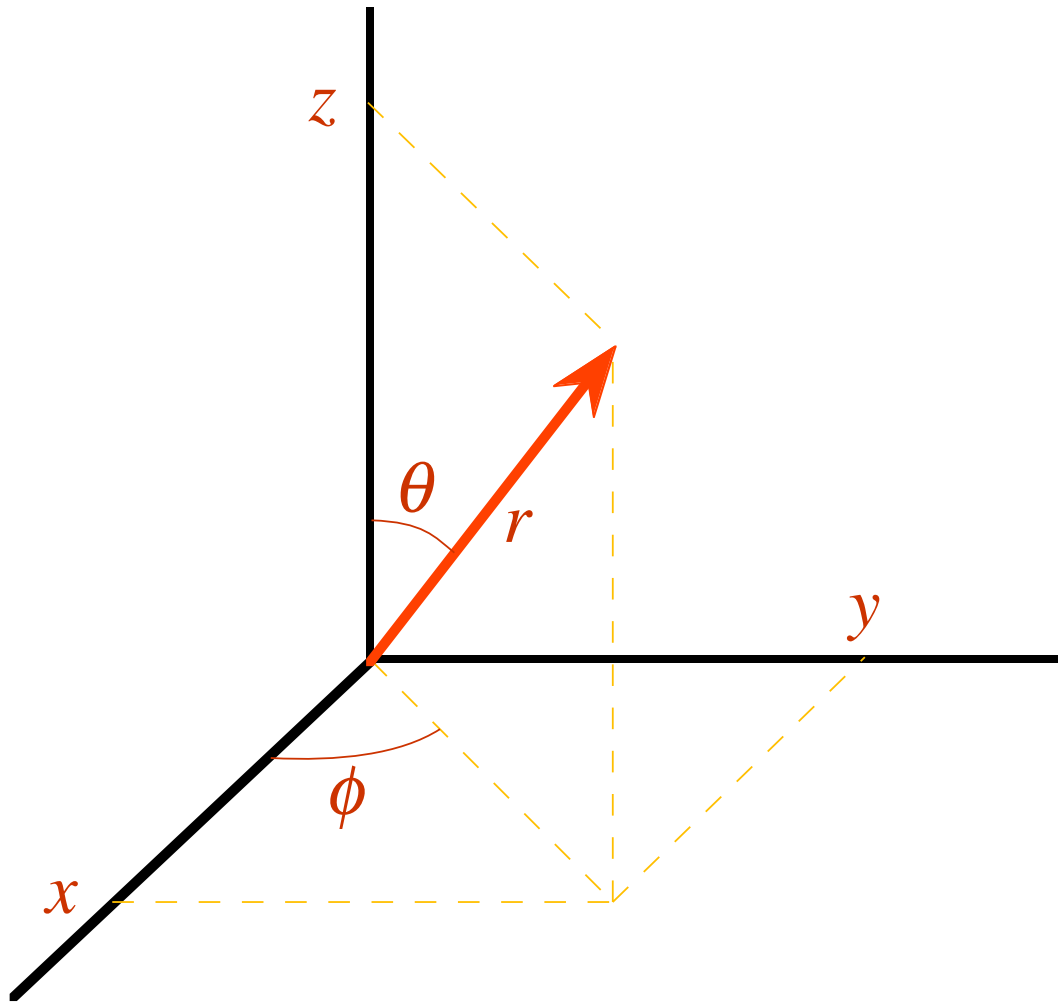
Ejemplo. Imprecisión mínima en la posición de partículas cuya imprecisión en la velocidad es del 1%

<i>Partícula</i>	<i>Masa (kg)</i>	<i>Velocidad ($m\ s^{-1}$)</i>	<i>Imprecisión mínima en la posición (m)</i>
Automóvil	1000	28 (100 km/h)	10^{-37}
Electrón del átomo de H ($n = 1$)	$9,11\ 10^{-31}$	$2,19\ 10^6$	$26\ 10^{-10}$ (26 Å, el radio de Bohr es 0,529 Å)





$n = 3$



(x, y, z) coordenadas cartesianas
 (r, θ, ϕ) coordenadas polares

$$z = r \cos \theta$$

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

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

$$\theta = \arccos(z/r)$$

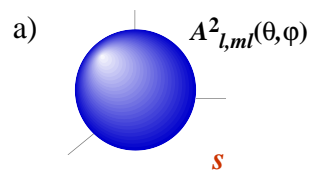
$$\phi = \arctg(y/x)$$

Tabla 1.6. Funciones radiales $R_{n,l}(r)$ normalizadas para átomos o iones monoeléctricos*

Orbital	n	l	$R_{n,l} =$	Constante	\times	Polinomio	\times	Exponencial
1s	1	0	$R_{1,0}$	$2Z^{3/2}$		1		e^{-Zr}
2s	2	0	$R_{2,0}$	$\frac{Z^{3/2}}{2\sqrt{2}}$		$(2 - Zr)$		$e^{-Zr/2}$
2p	2	1	$R_{2,0}$	$\frac{Z^{3/2}}{2\sqrt{6}}$		Zr		$e^{-Zr/2}$
3s	3	0	$R_{3,0}$	$\frac{2Z^{3/2}}{81\sqrt{3}}$		$(27 - Zr + Z^2r^2)$		$e^{-Zr/3}$
3p	3	1	$R_{3,1}$	$\frac{4Z^{3/2}}{81\sqrt{6}}$		$(6Zr - Z^2r^2)$		$e^{-Zr/3}$
3d	3	2	$R_{3,2}$	$\frac{4Z^{3/2}}{81\sqrt{30}}$		Z^2r^2		$e^{-Zr/3}$
4s	4	0	$R_{4,0}$	$\frac{Z^{3/2}}{768}$		$(192 - 144Zr + 24Z^2r^2 - Z^3r^3)$		$e^{-Zr/4}$
4p	4	1	$R_{4,1}$	$\frac{Z^{3/2}}{256\sqrt{15}}$		$(80Zr - 20Z^2r^2 + Z^3r^3)$		$e^{-Zr/4}$
4d	4	2	$R_{4,2}$	$\frac{Z^{3/2}}{768\sqrt{5}}$		$(12Z^2r^2 - Z^3r^3)$		$e^{-Zr/4}$
4f	4	3	$R_{4,3}$	$\frac{Z^{3/2}}{768\sqrt{35}}$		Z^3r^3		$e^{-Zr/4}$
	n	l	$R_{n,l} = \sum_{x=l}^{n-1} 1$	N_x		r^x		$e^{-Zr/n}$

* Las funciones se dan en base al sistema de unidades atómicas (es decir, r en unidades de a_0).

Parte Angular



Parte Radial

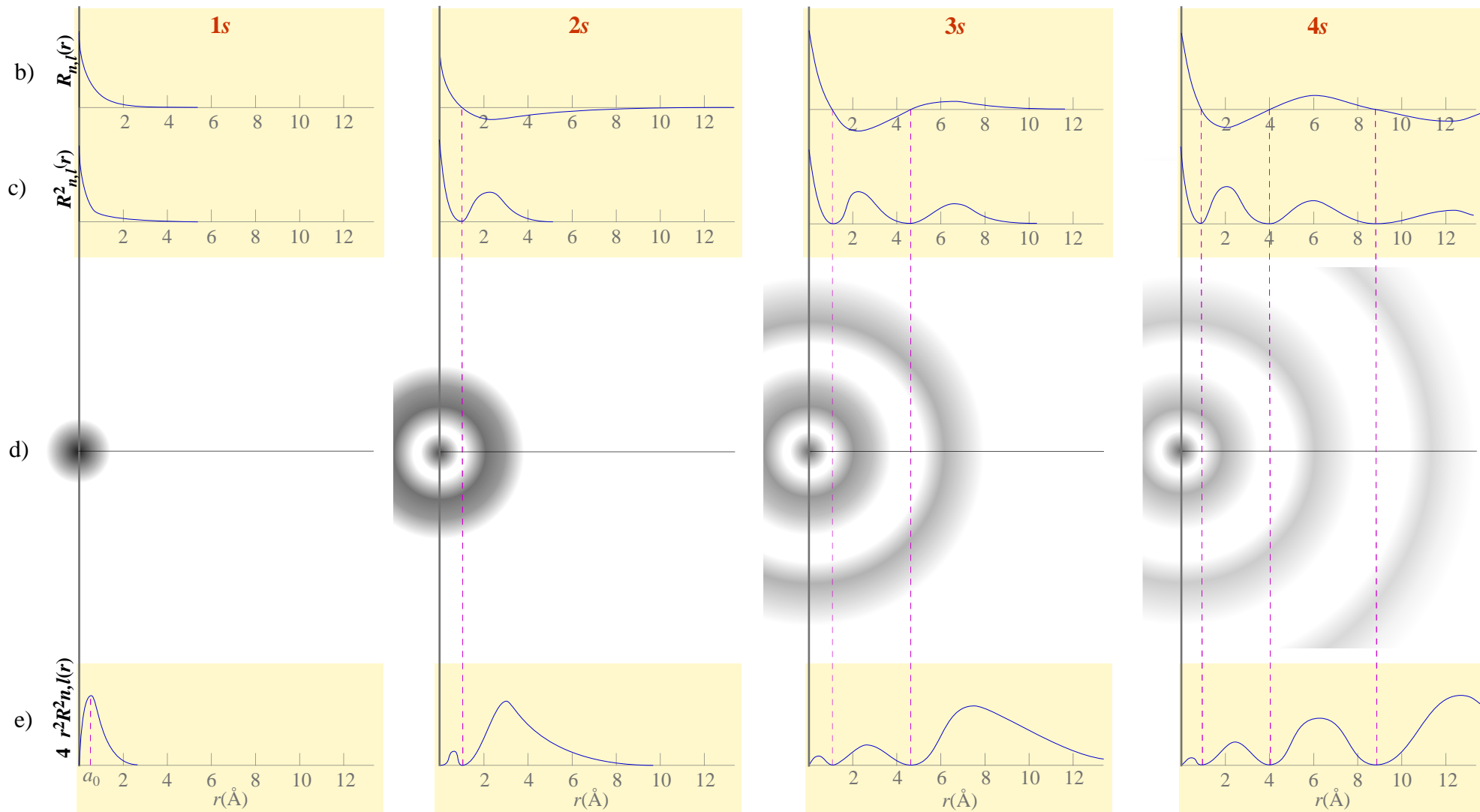
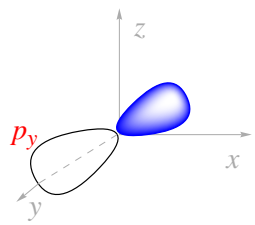
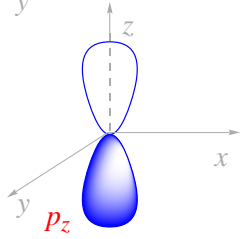
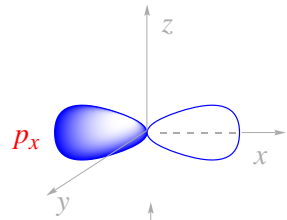


Tabla 1.7. Funciones angulares A_{l,m_l} normalizadas para átomos o iones monoelectrónicos

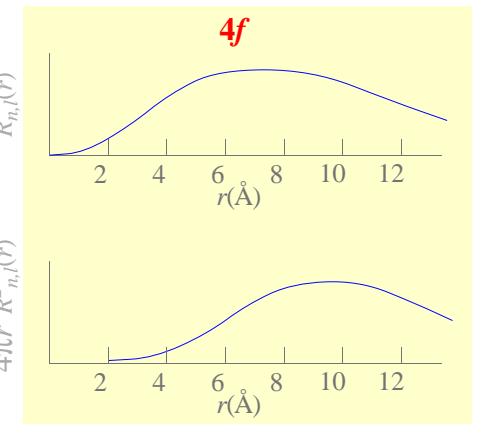
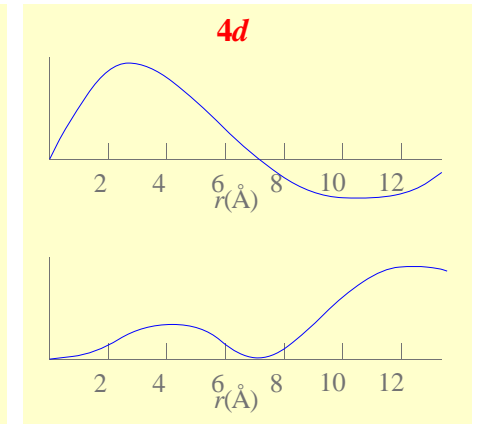
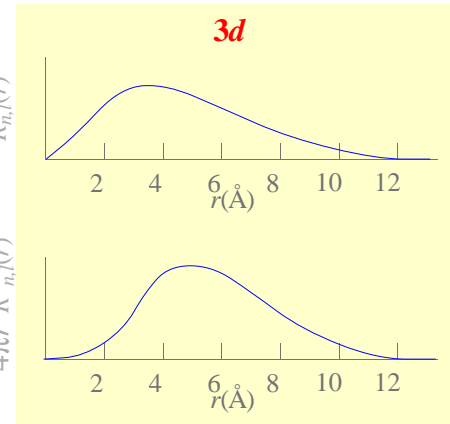
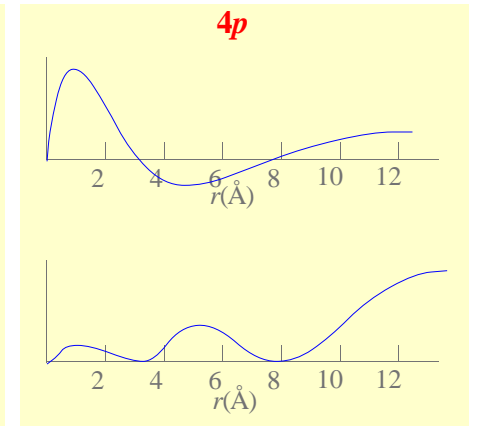
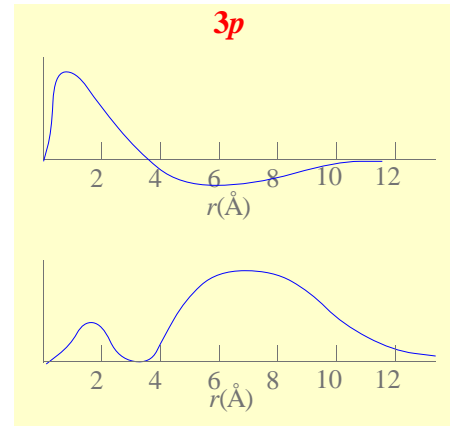
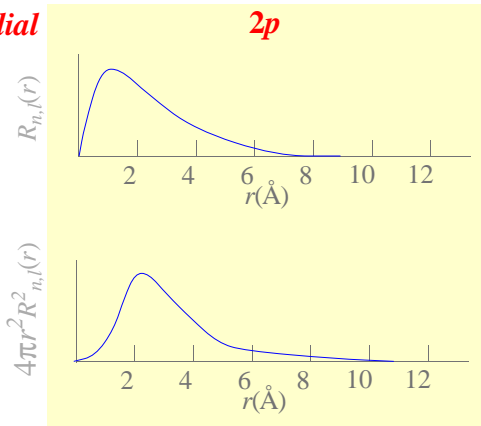
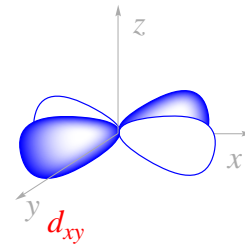
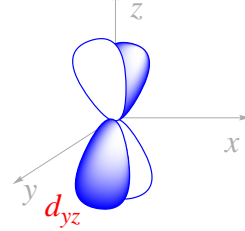
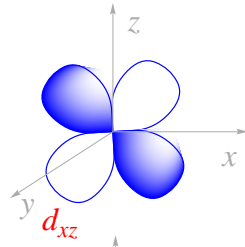
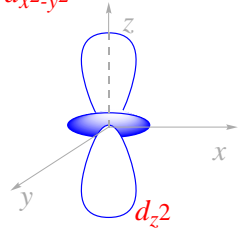
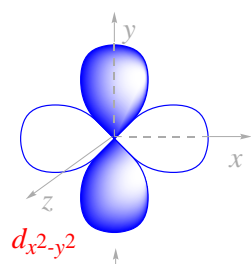
Orbital	$A_{l,m_l}(\theta, \phi)^*$	$A_{l,m_l}(x, y, z)^{**}$
s	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
p_z	$\frac{\sqrt{3}}{2\sqrt{\pi}} \cos \theta$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (z/r)$
p_x	$\frac{\sqrt{3}}{2\sqrt{\pi}} \text{sen } \theta \cos \phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (x/r)$
p_y	$\frac{\sqrt{3}}{2\sqrt{\pi}} \text{sen } \theta \text{sen } \phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (y/r)$
d_{z^2}	$\frac{\sqrt{5}}{4\sqrt{\pi}} (3 \cos^2 \theta - 1)$	$\frac{\sqrt{5}}{4\sqrt{\pi}} [(2z^2 - x^2 - y^2)/r^2]$
d_{zx}	$\frac{\sqrt{15}}{2\sqrt{\pi}} \cos \theta \text{sen } \theta \cos \phi$	$\frac{\sqrt{15}}{2\sqrt{\pi}} (zx/r^2)$
d_{zy}	$\frac{\sqrt{15}}{2\sqrt{\pi}} \cos \theta \text{sen } \theta \text{sen } \phi$	$\frac{\sqrt{15}}{2\sqrt{\pi}} (zy/r^2)$
$d_{x^2 - y^2}$	$\frac{\sqrt{15}}{4\sqrt{\pi}} \text{sen}^2 \theta (2 \cos^2 \phi - 1)$	$\frac{\sqrt{15}}{4\sqrt{\pi}} [(x^2 - y^2)/r^2]$
d_{xy}	$\frac{\sqrt{15}}{2\sqrt{\pi}} \text{sen}^2 \theta \text{sen } \phi \cos \phi$	$\frac{\sqrt{15}}{2\sqrt{\pi}} (xy/r^2)$
f_{z^3}	$\frac{\sqrt{7}}{4\sqrt{\pi}} (5 \cos^3 \theta - 3 \cos \theta)$	$\frac{\sqrt{7}}{4\sqrt{\pi}} [(2z^3 - 3x^2z - 3y^2z)/r^3]$
f_{z^2x}	$\frac{\sqrt{42}}{8\sqrt{\pi}} (5 \cos^2 \theta - 1) \text{sen } \theta \cos \phi$	$\frac{\sqrt{42}}{8\sqrt{\pi}} [(4z^2x - x^3 - y^2x)/r^3]$
f_{z^2y}	$\frac{\sqrt{42}}{8\sqrt{\pi}} (5 \cos^2 \theta - 1) \text{sen } \theta \text{sen } \phi$	$\frac{\sqrt{42}}{8\sqrt{\pi}} [(4z^2y - x^2y - y^3)/r^3]$
$f_{z(x^2 - y^2)}$	$\frac{\sqrt{105}}{4\sqrt{\pi}} \cos \theta \text{sen}^2 \theta (2 \cos^2 \phi - 1)$	$\frac{\sqrt{105}}{4\sqrt{\pi}} [z(x^2 - y^2)/r^3]$
f_{zxy}	$\frac{\sqrt{105}}{2\sqrt{\pi}} \cos \theta \text{sen}^2 \theta \cos \phi \text{sen } \phi$	$\frac{\sqrt{105}}{2\sqrt{\pi}} (zxy/r^3)$
f_{x^3}	$\frac{\sqrt{70}}{8\sqrt{\pi}} \text{sen}^3 \theta (4 \cos^3 \phi - 3 \cos \phi)$	$\frac{\sqrt{70}}{8\sqrt{\pi}} [(x^3 - 3xy^2)/r^3]$
f_{y^3}	$\frac{\sqrt{70}}{8\sqrt{\pi}} \text{sen}^3 \theta (3 \text{sen } \phi - 4 \text{sen}^3 \phi)$	$\frac{\sqrt{70}}{8\sqrt{\pi}} [(-y^3 + 3x^2y)/r^3]$

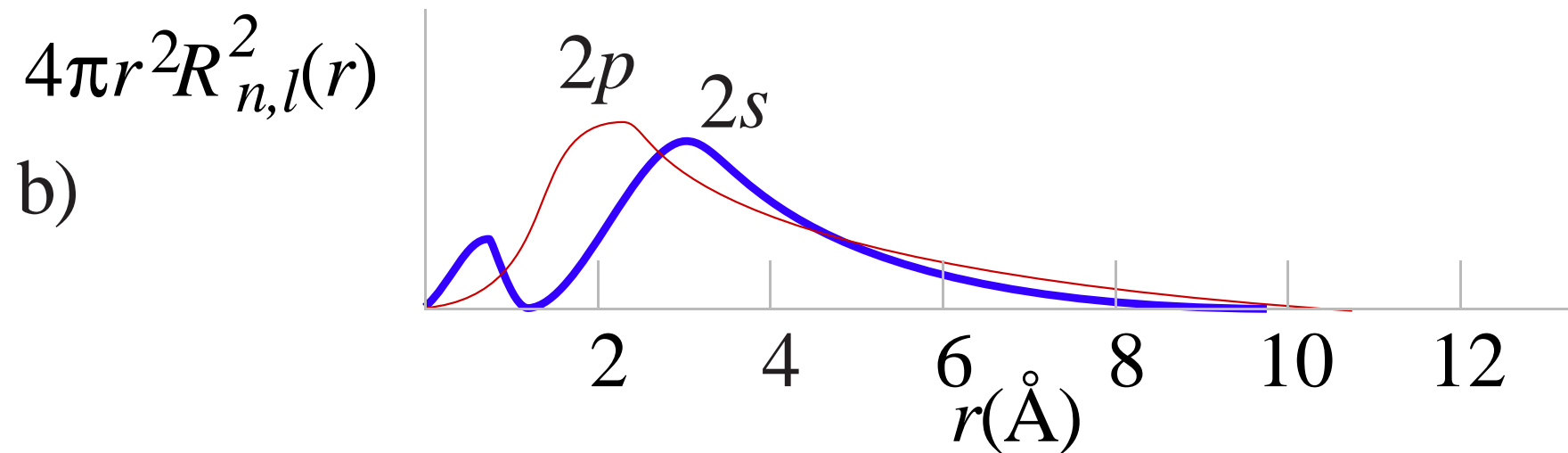
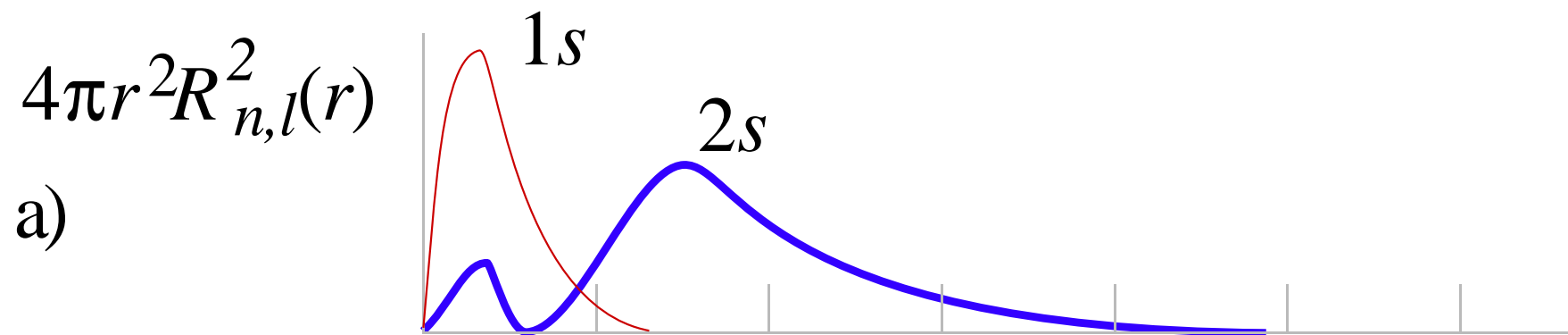
* Funciones en el sistema de coordenadas polares esféricas. ** Funciones en el sistema de coordenadas cartesiano.

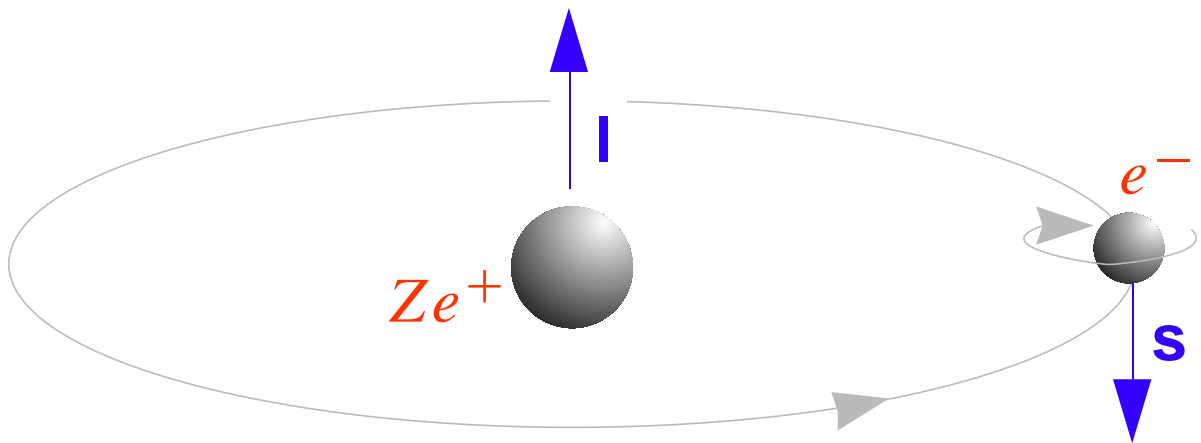
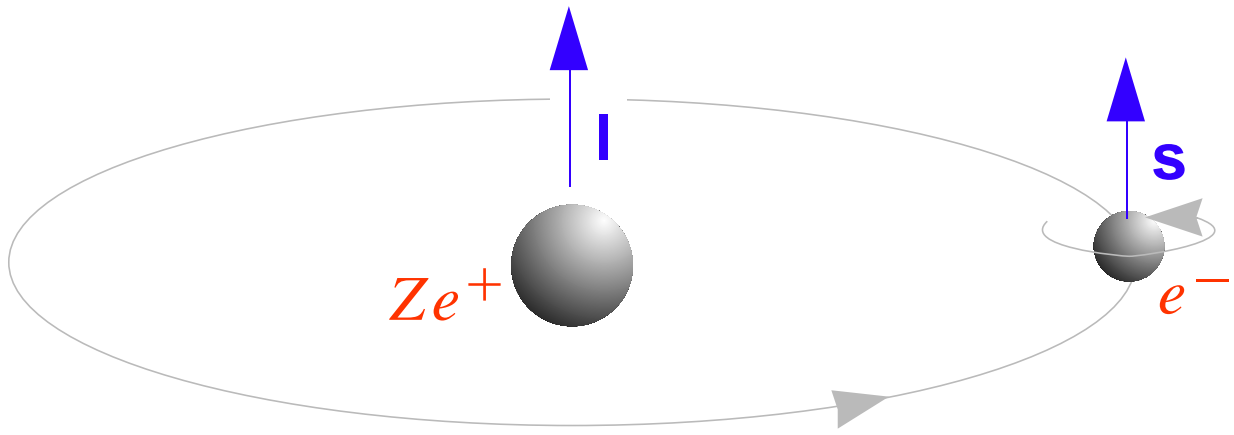
Parte Angular



Parte Radial







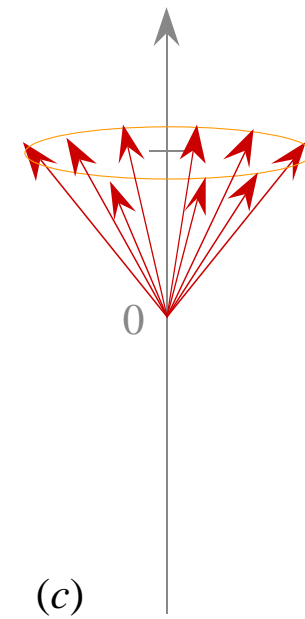
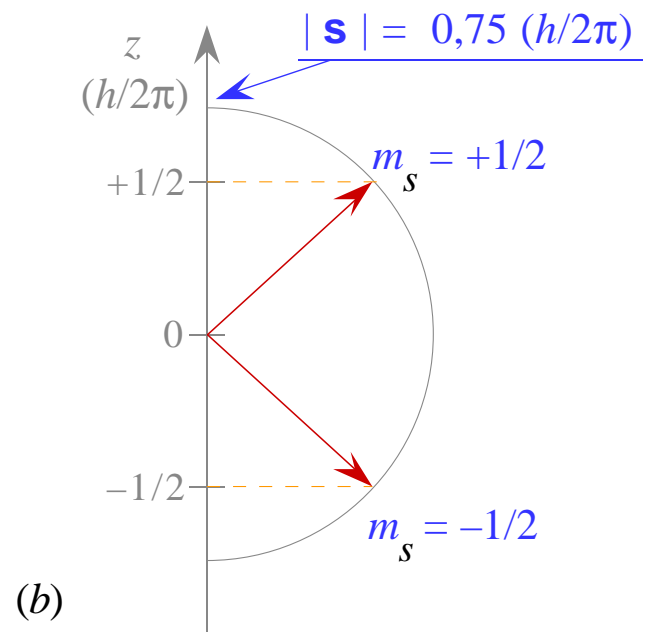
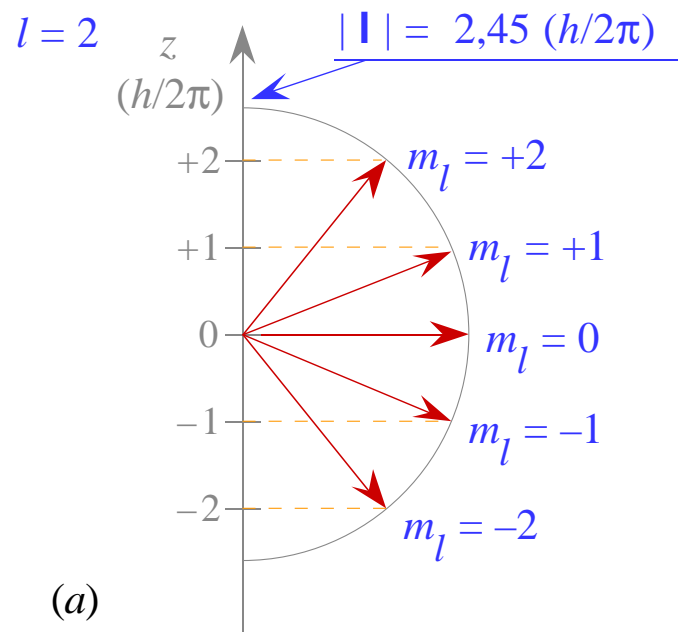
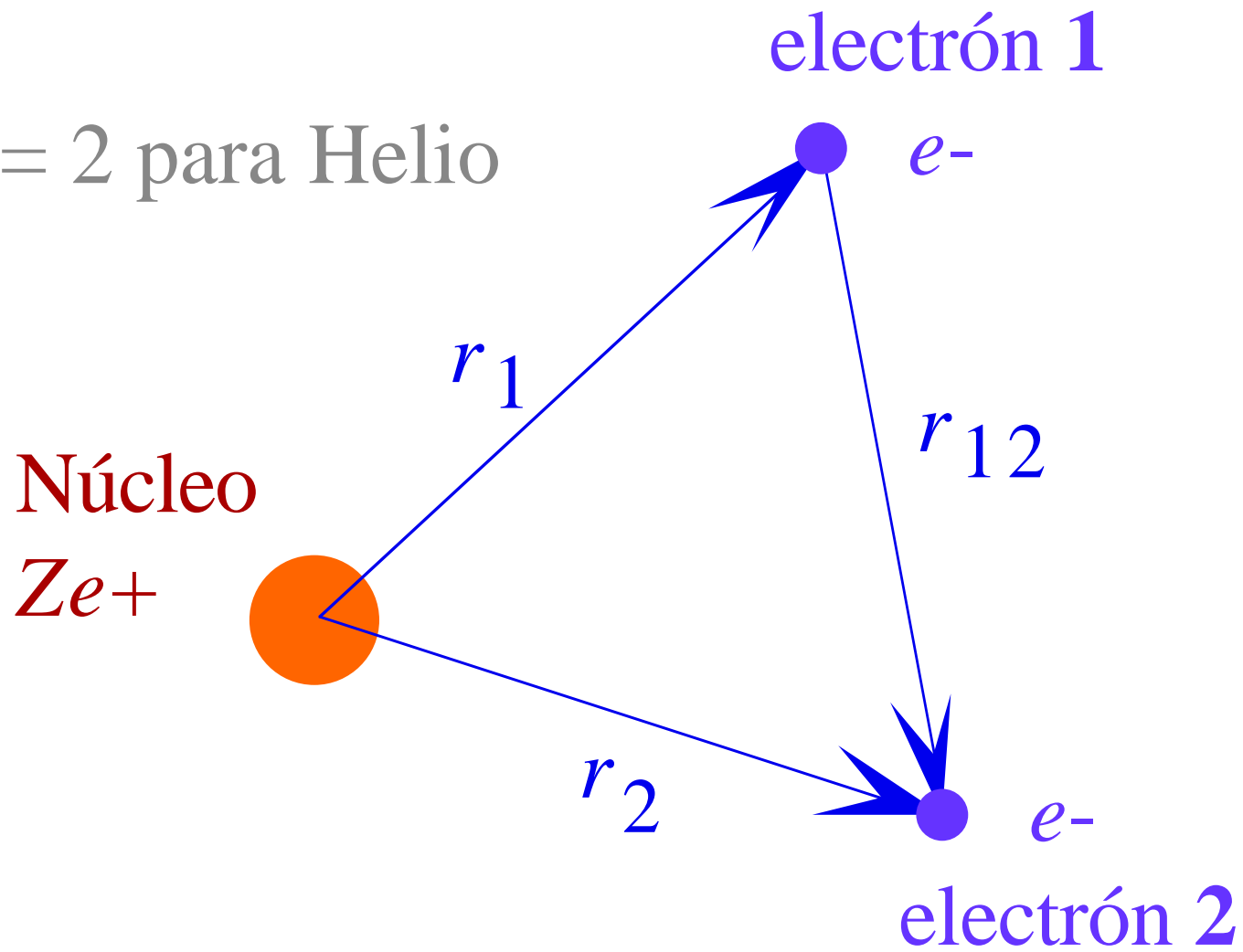


Tabla 1.8. Niveles de energía de un electrón en un orbital del hidrógeno, considerando la interacción espín-órbita

<i>Orbital</i>	<i>l</i>	<i>s</i>	$j = l + s, \dots, l - s $	<i>Nº de niveles de energía</i>	<i>Nº de microestados (2j + 1)</i>
<i>s</i>	0	1/2	1/2	1	2
<i>p</i>	1	1/2	3/2, 1/2	2	4 + 2 = 6
<i>d</i>	2	1/2	5/2, 3/2	2	6 + 4 = 10
<i>f</i>	3	1/2	7/2, 5/2	2	8 + 6 = 14

$Z = 2$ para Helio



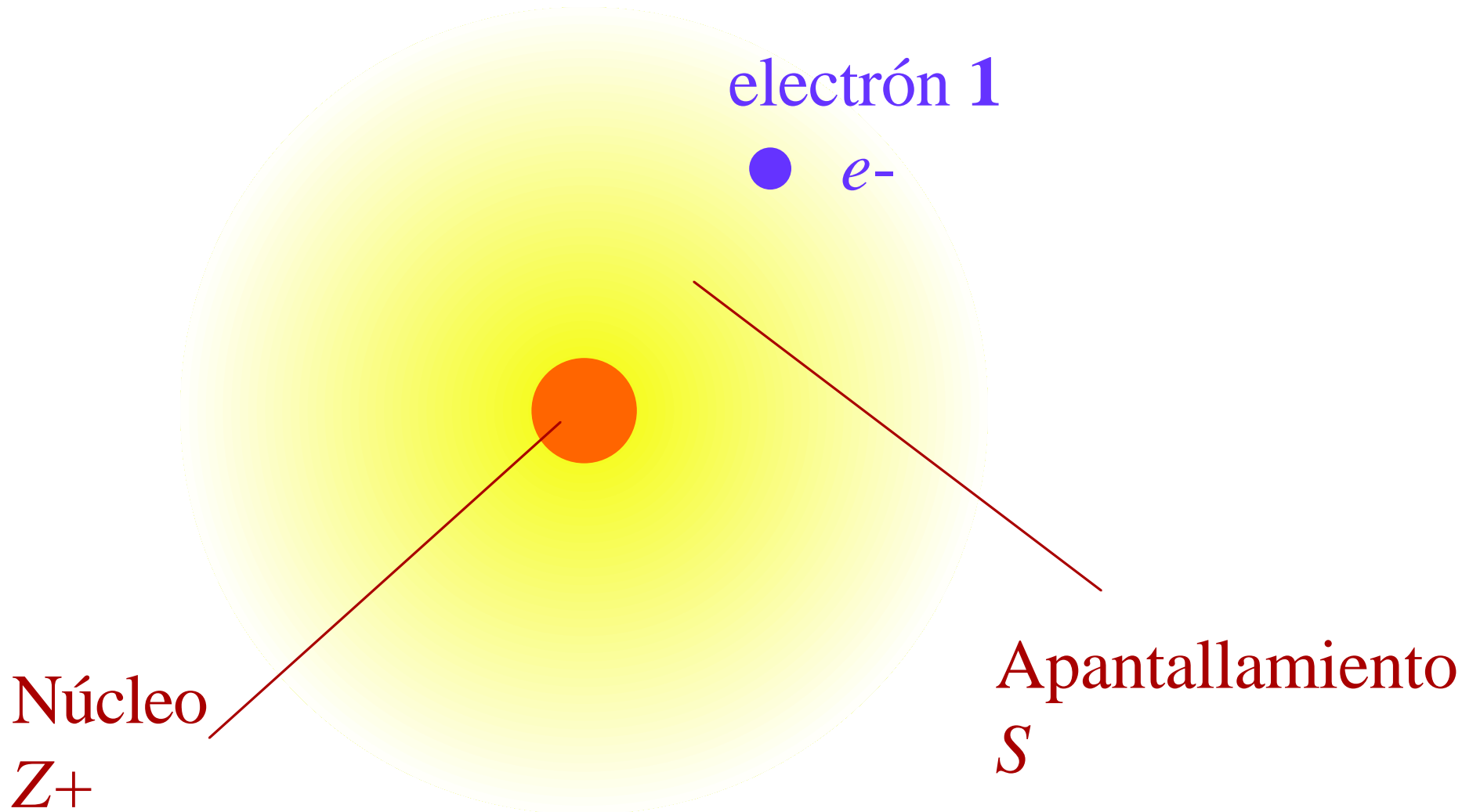
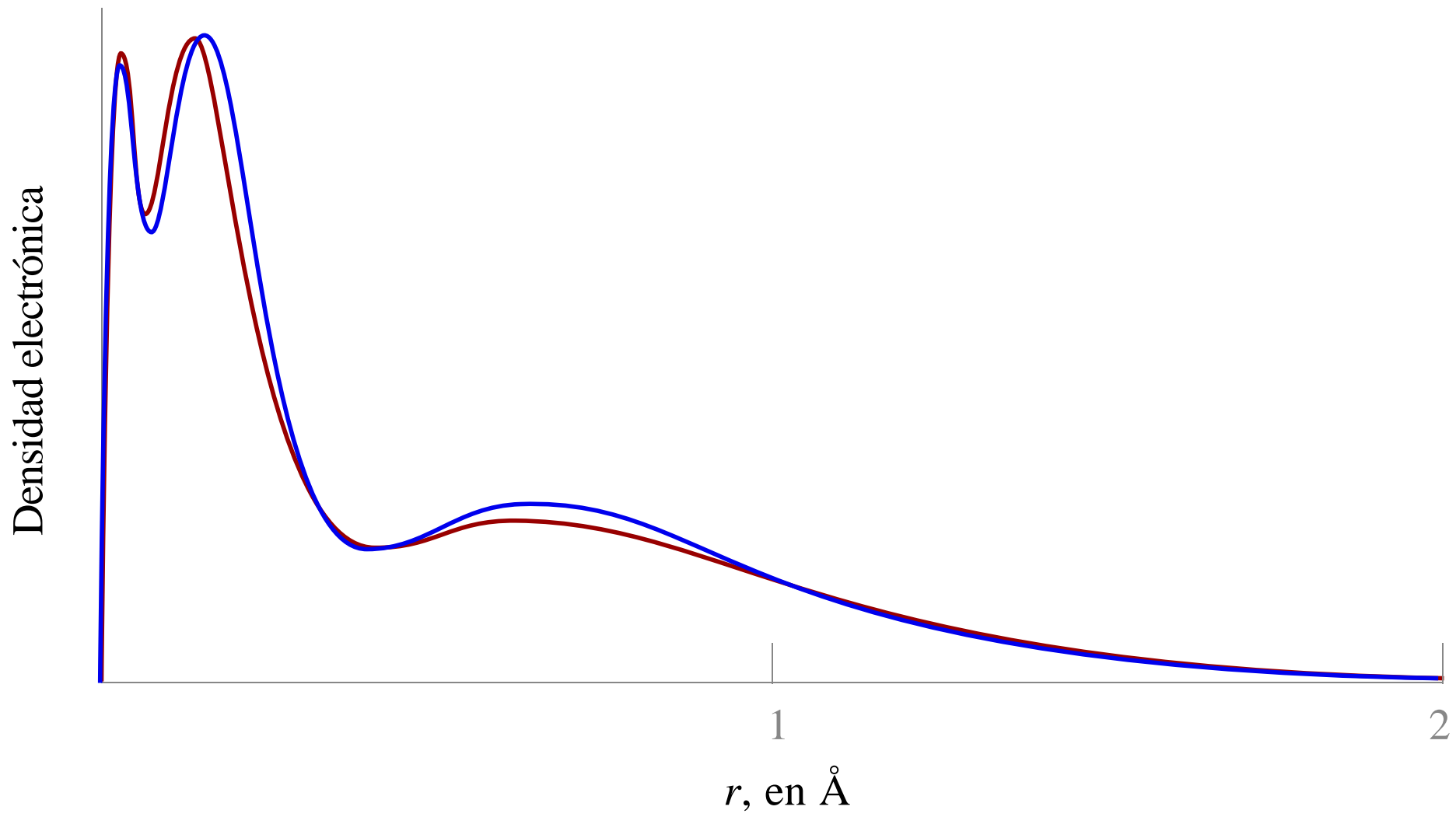


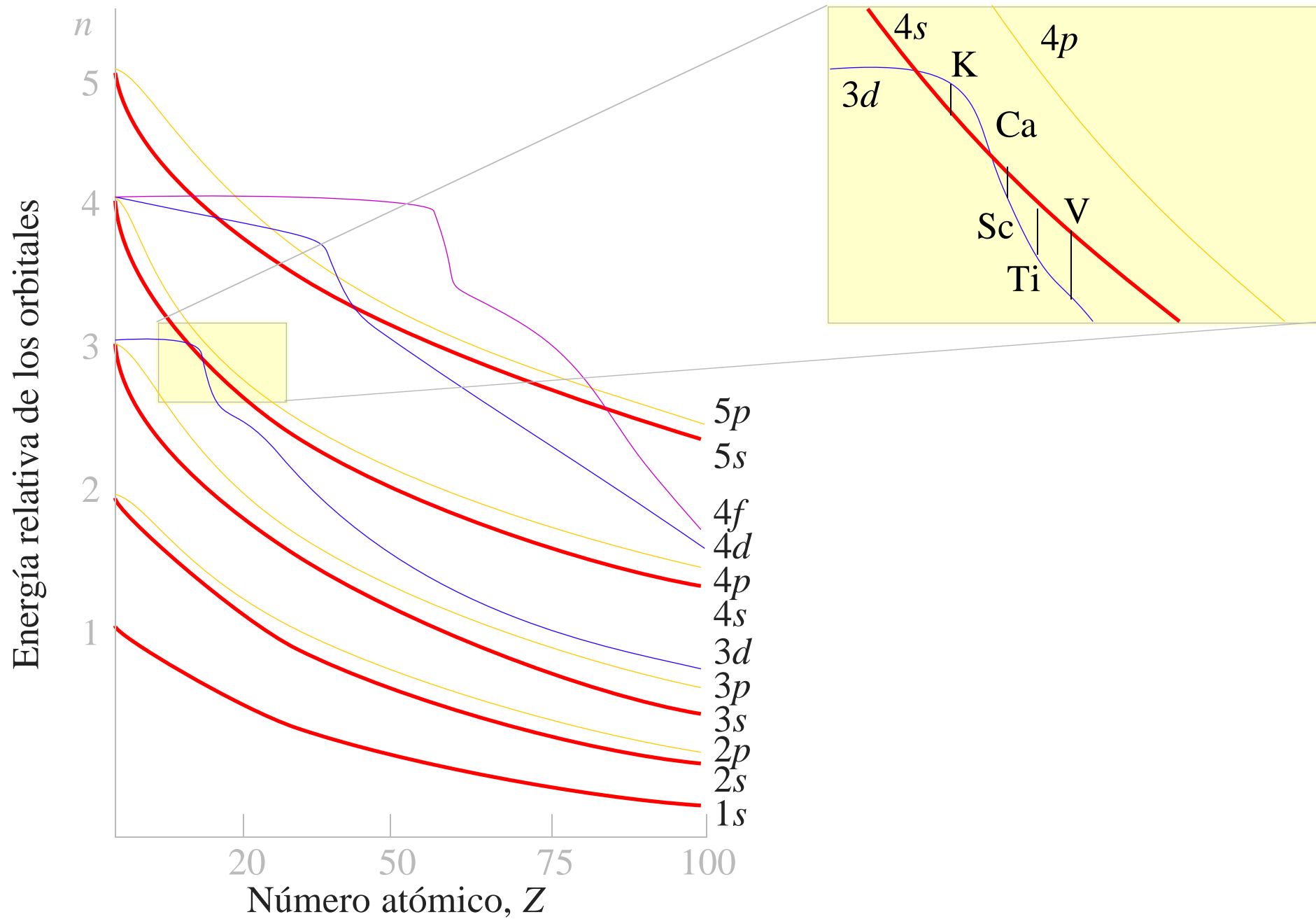
Tabla 1.9 (parcial). Cargas Nucleares Efectivas de los elementos del 1 al 36

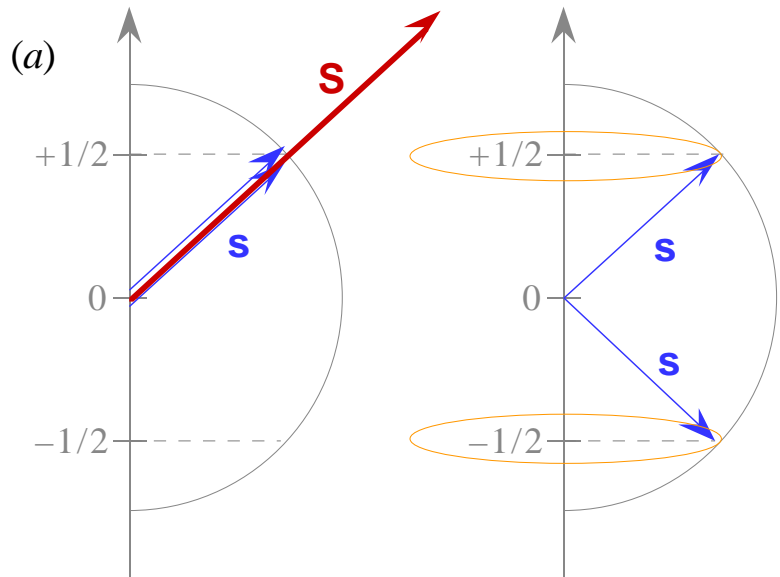
Elemento	1s	2s	2p	3s	3p	4s
H	1,000					
He	1,688					
Li	2,691	1,279				
Be	3,685	1,912				
B	4,680	2,576	2,421			
C	5,673	3,217	3,136			
N	6,665	3,847	3,834			
O	7,658	4,492	4,453			
F	8,650	5,128	5,100			
Ne	9,642	5,758	5,758			
Na	10,626	6,571	6,802	2,507		
Mg	11,619	7,392	7,826	3,308		
Al	12,591	8,214	8,963	4,117	4,066	
Si	13,575	9,020	9,945	4,903	4,285	
P	14,558	9,825	10,961	5,642	4,886	
S	15,541	10,629	11,977	6,367	5,482	
Cl	16,524	11,430	12,993	7,068	6,116	
Ar	17,508	12,230	14,008	7,757	6,764	
K	18,490	13,006	15,027	8,680	7,726	3,495

Tabla 1.10. Energías calculadas para el helio en su estado fundamental a partir de funciones de onda aproximadas

Tipo de función de onda		Energía (en eV)
1	Producto de orbitales del He ⁺ (aprox. orbital)	-74,83
2	Producto de orbitales con Z* fijada por el método SCF	-77,48
3	Producto de funciones más apropiado	-77,870917
4	Función no orbitalaria de Pekeris (combinación lineal de 1078 términos)	-79,00946912
	Valor experimental (I₁ + I₂)	-79,014

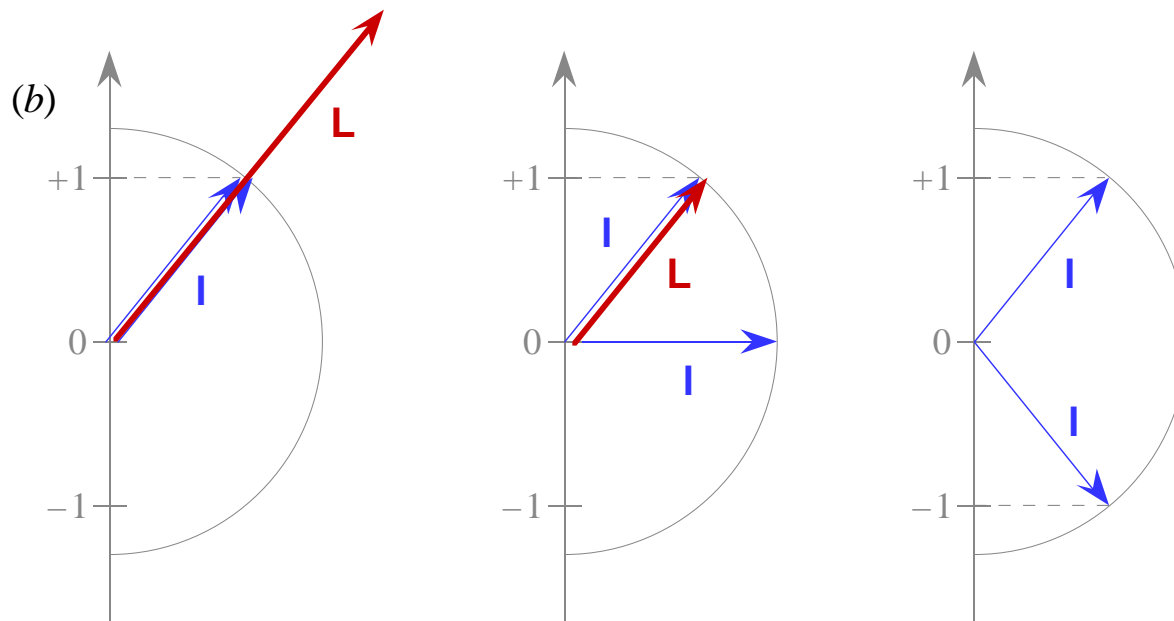






$s = 1/2$
 $S = 1$
 $M_S = +1, 0, -1$

$s = 1/2$
 $S = 0$
 $M_S = 0$



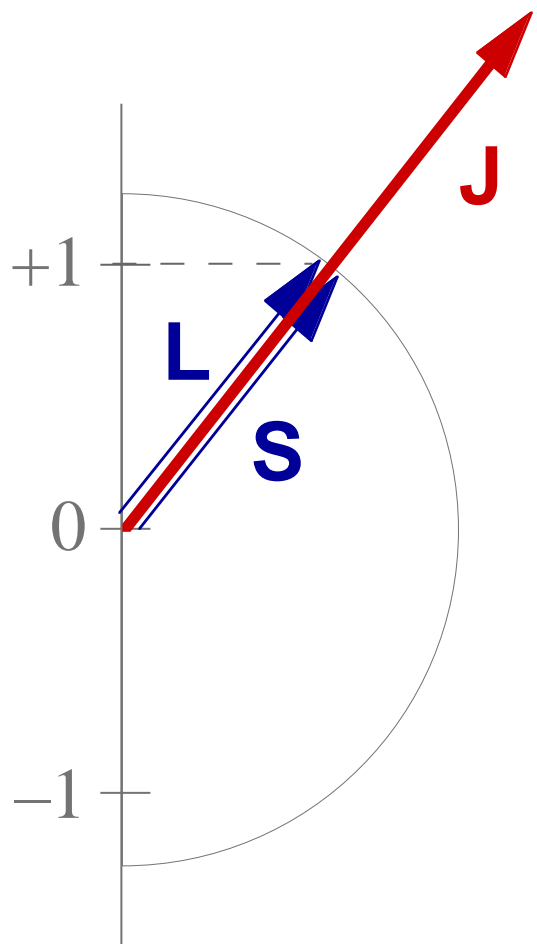
$l = 1$
 $L = 2$
 $M_L = +2, +1, 0, -1, -2$

$l = 1$
 $L = 1$
 $M_L = +1, 0, -1$

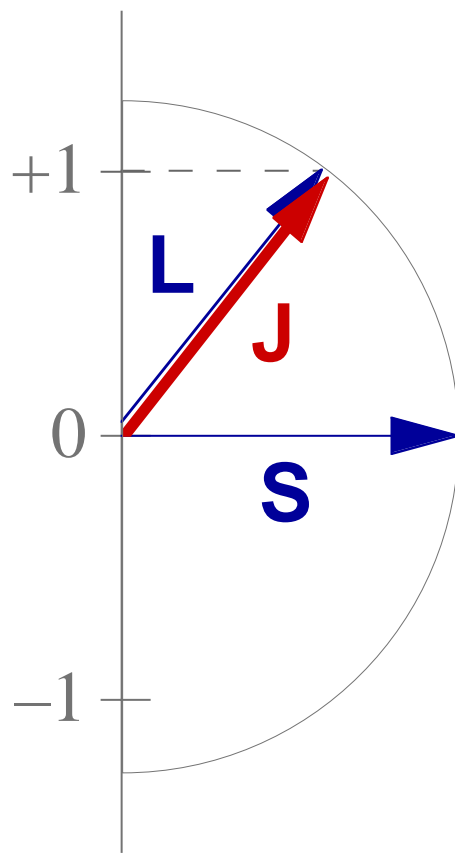
$l = 1$
 $L = 0$
 $M_L = 0$

Tabla 1.12. Términos Russell–Saunders para algunas configuraciones

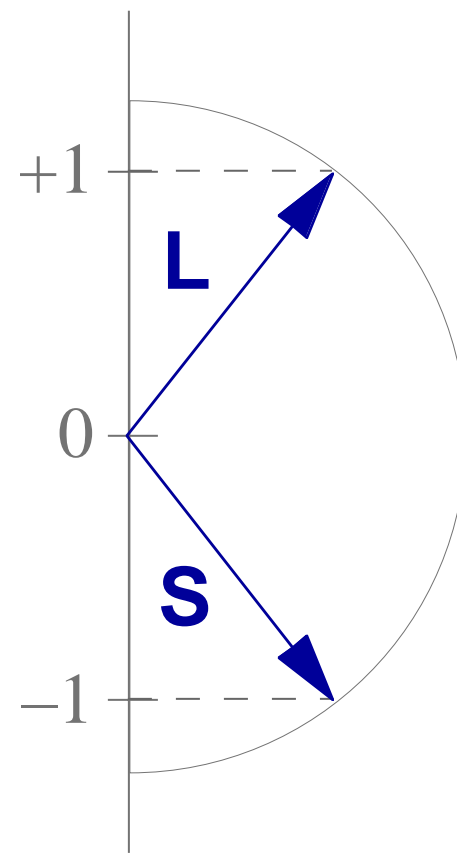
Configuración	Términos	Término fundamental
s^1	2S	2S
s^2	1S	1S
p^1 y p^5	2P	2P
p^2 y p^4	$^1S, ^1D, ^3P$	3P
p^3	$^2P, ^2D, ^4S$	4S
p^6	1S	1S
d^1 y d^9	2D	2D
d^2 y d^8	$^1S, ^1D, ^1G, ^3P, ^3F$	3F
d^3 y d^7	$^2P, ^2D(2), ^2F, ^2G, ^2H, ^4P, ^4F$	4F
d^4 y d^6	$^1S(2), ^1D(2), ^1F, ^1G(2), ^1I, ^3P(2), ^3D, ^3F(2), ^3G, ^3H, ^5D$	5D
d^5	$^2S, ^2P, ^2D(3), ^2F(2), ^1I, ^2G(2), ^3H, ^2I, ^4P, ^4D, ^4F, ^4G, ^6S$	6S



(a)
 $M_S = 1$
 $J = 2$



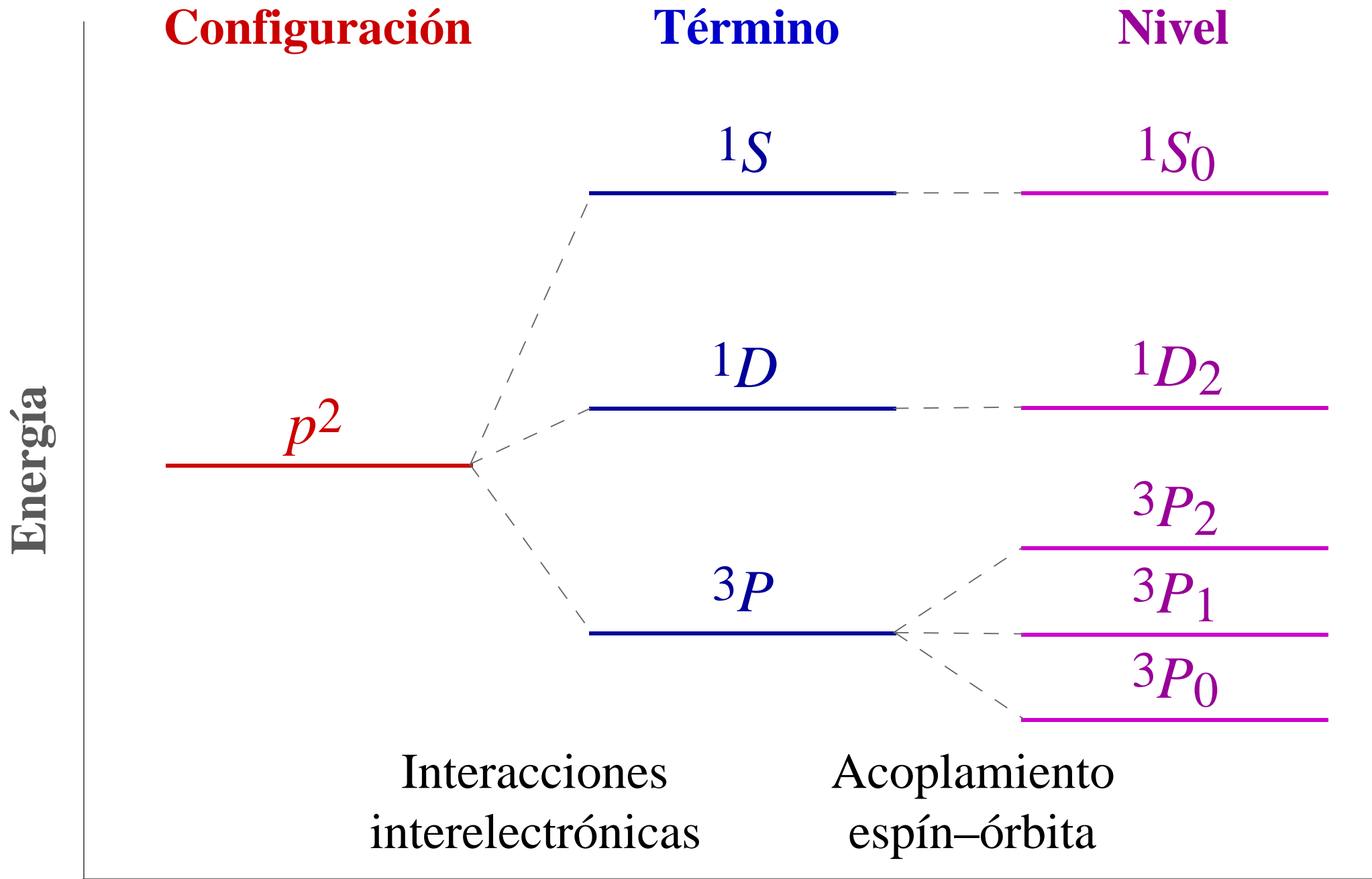
(b)
 $M_S = 0$
 $J = 1$

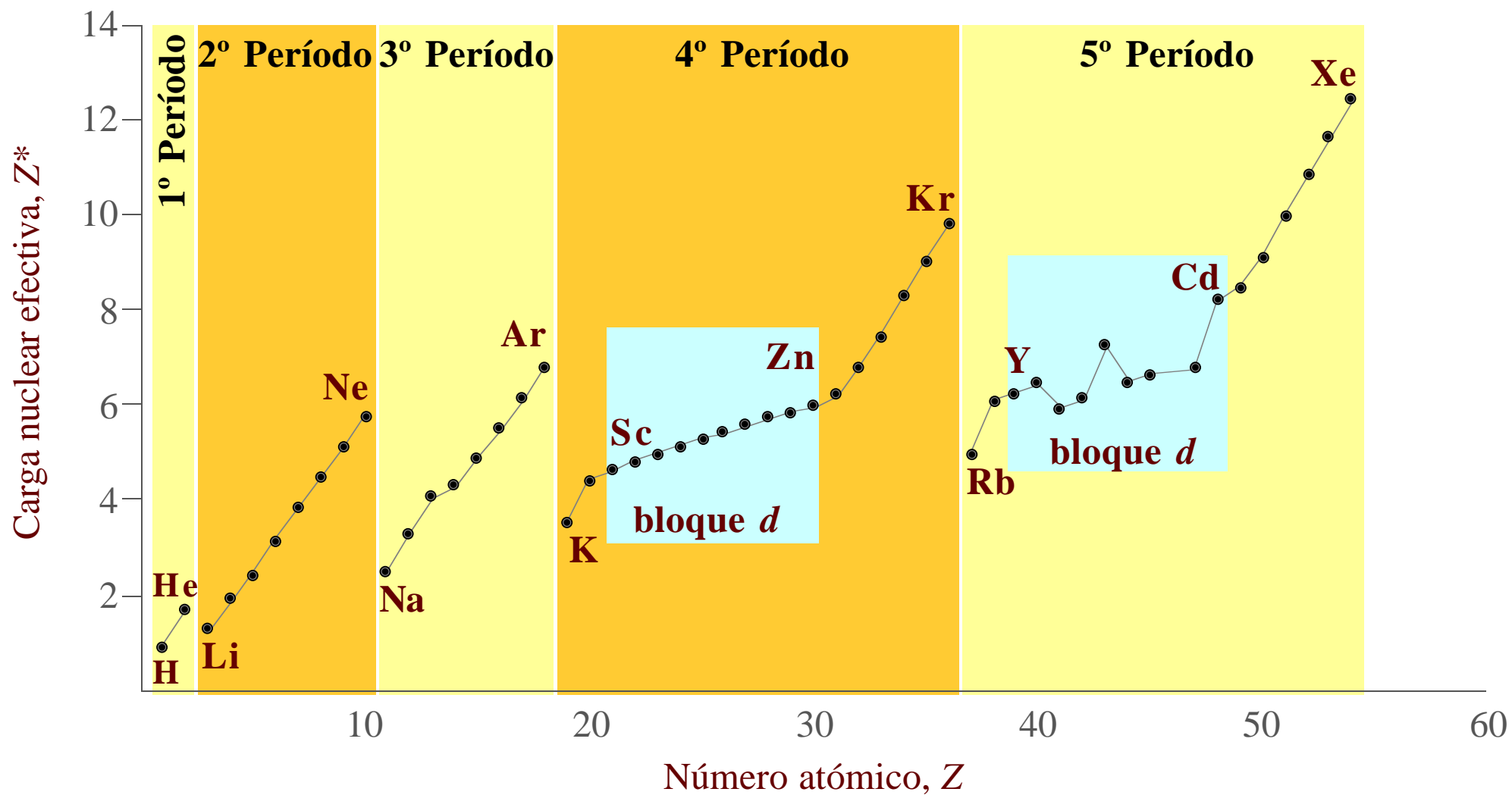


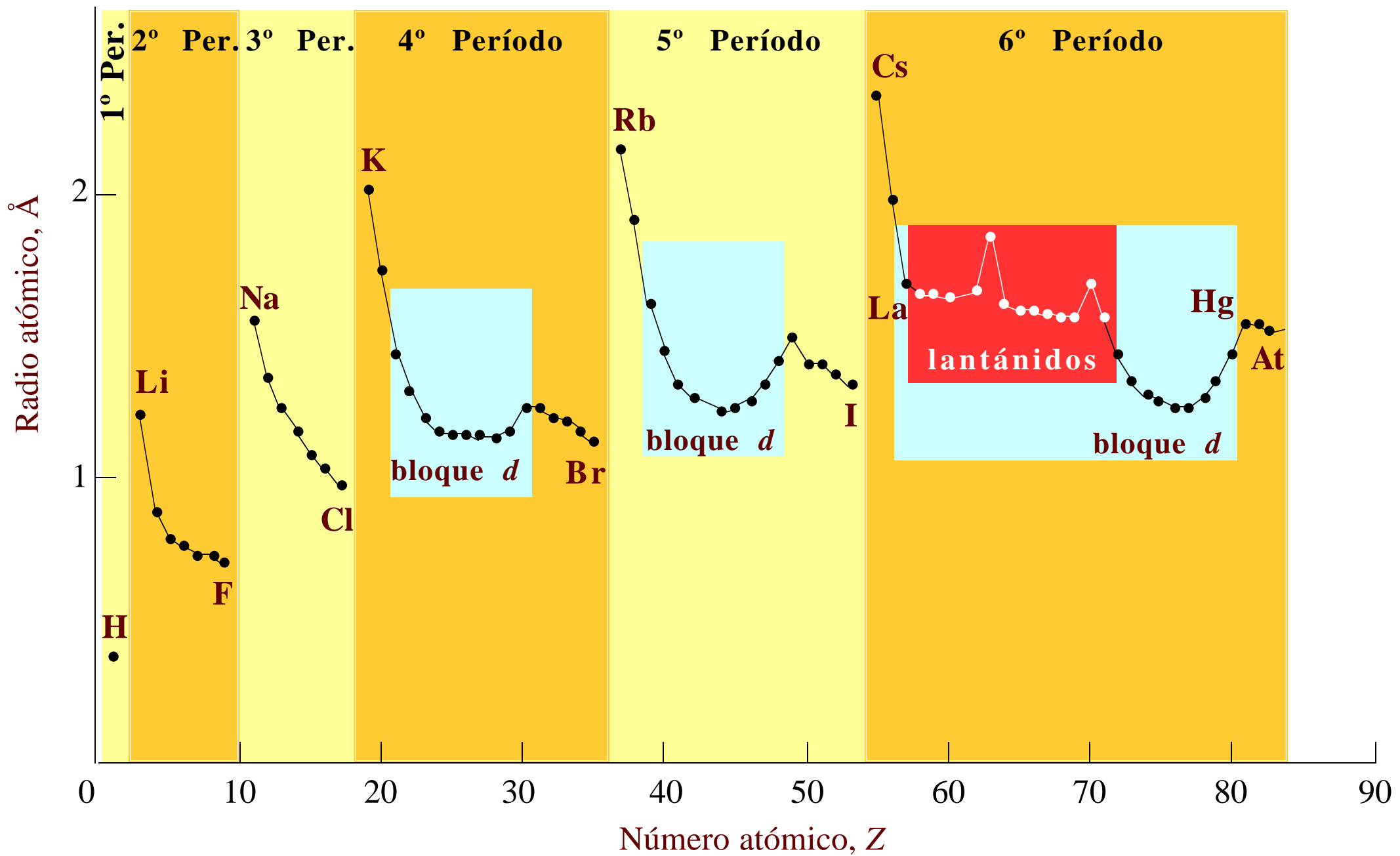
(c)
 $M_S = -1$
 $J = 0$

Tabla 1.13. Niveles de energía de una configuración p^2

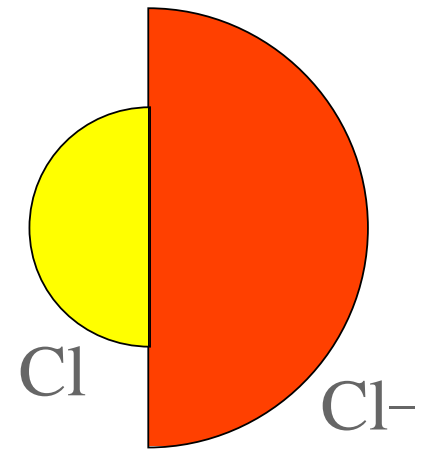
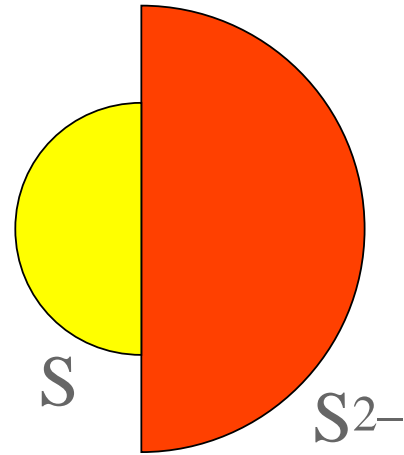
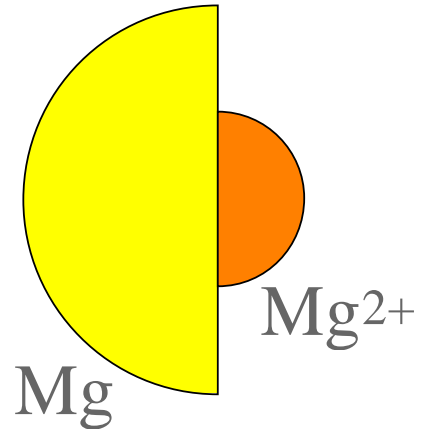
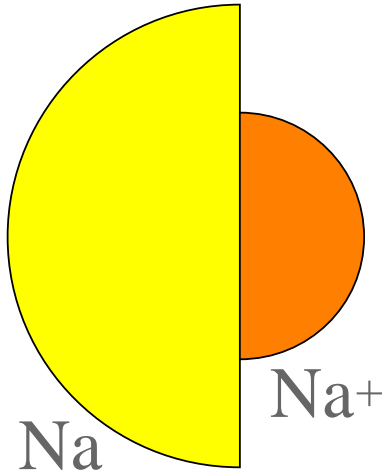
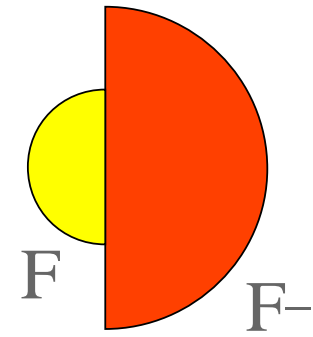
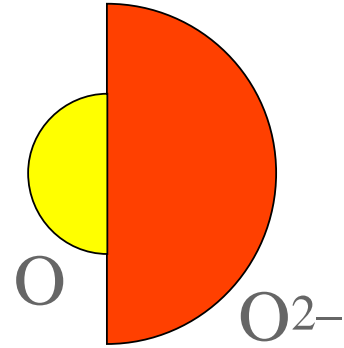
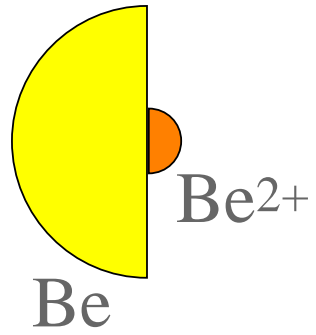
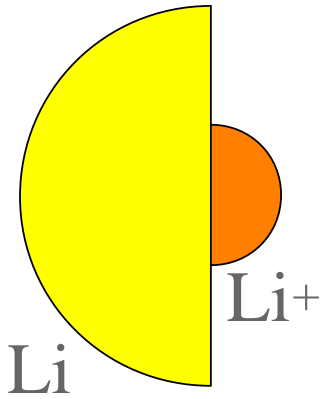
Término	Degeneración tno.	$J = L+S, \dots, L-S$	Símbolo nivel	Orientaciones de J	Degeneración nivel ($2J + 1$)
$1D$	5	$J = 2$	$1D_2$	$M_J = +2, +1, 0, -1, -2$	5 microestados
$3P$	9	$J = 2, 1, 0$	$3P_2$	$M_J = +2, +1, 0, -1, -2$	5 microestados
			$3P_1$	$M_J = +1, 0, -1$	3 microestados
			$3P_0$	$M_J = 0$	1 microestado
$1S$	1	$J = 0$	$1S_0$	$M_J = 0$	1 microestado

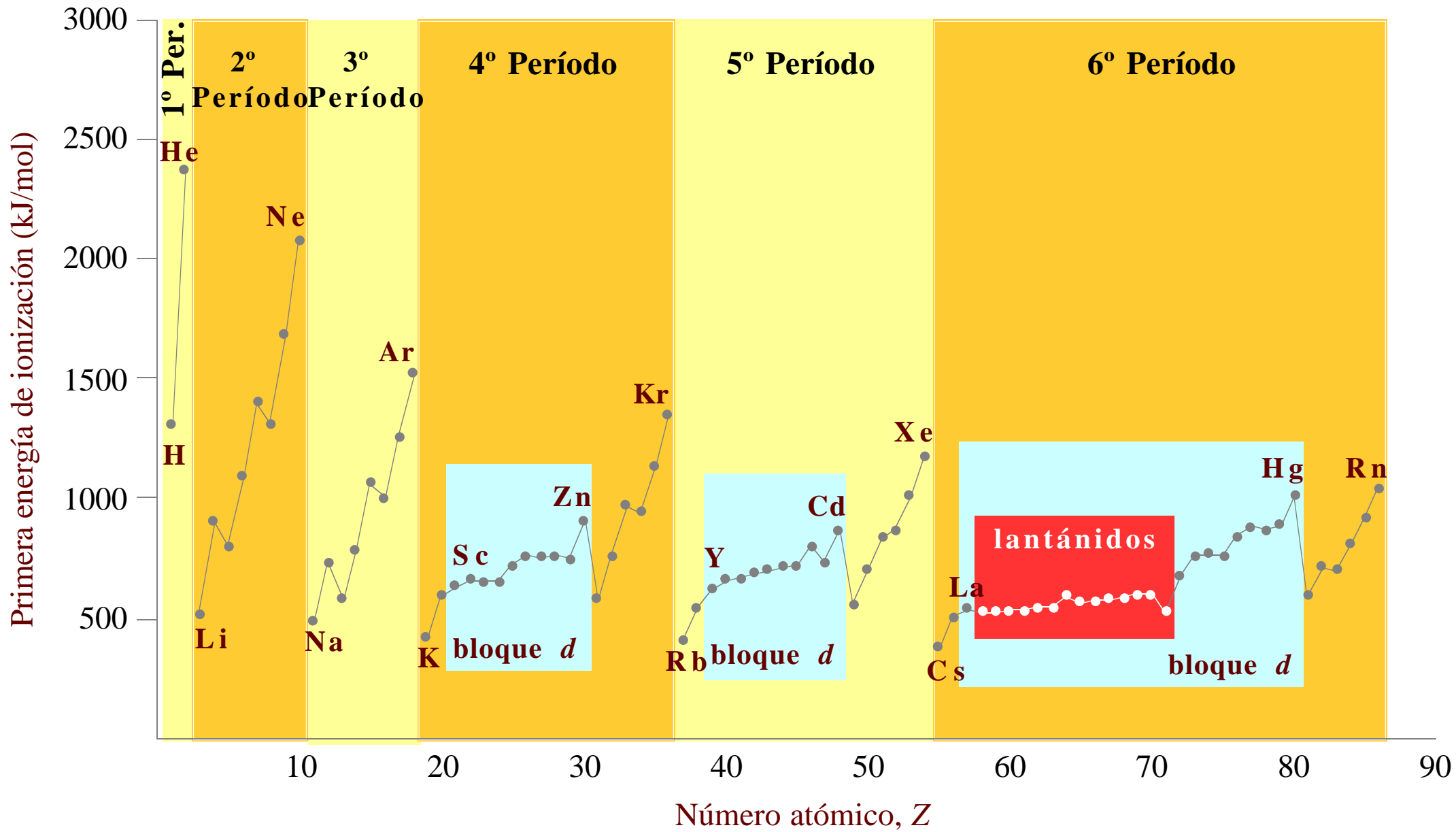




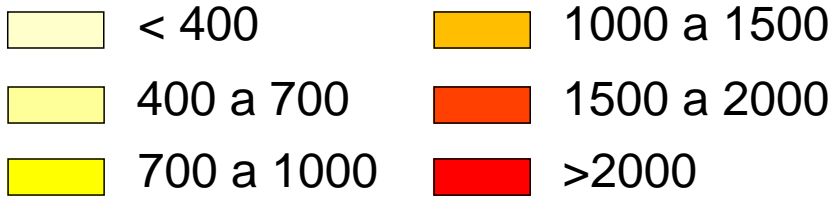


1Å





1												13						18
H 1310																		He 2370
Li 519	Be 900											B 799	C 1090	N 1400	O 1310	F 1680	Ne 2080	
Na 494	Mg 736	3	4	5	6	7	8	9	10	11	12	Al 577	Si 786	P 1060	S 1000	Cl 1260	Ar 1520	
K 418	Ca 590	Sc 631	Ti 658	V 650	Cr 652	Mn 717	Fe 759	Co 758	Ni 757	Cu 745	Zn 906	Ga 577	Ge 762	As 966	Se 941	Br 1140	Kr 1350	
Rb 402	Sr 548	Y 617	Zr 661	Nb 664	Mo 685	Tc 702	Ru 711	Rh 720	Pd 804	Ag 731	Cd 868	In 556	Sn 707	Sb 833	Te 870	I 1010	Xe 1170	
Cs 376	Ba 502	La 538	Hf 681	Ta 761	W 770	Re 760	Os 840	Ir 880	Pt 870	Au 890	Hg 1007	Tl 590	Pb 716	Bi 703	Po 812	At 920	Rn 1040	
Fr	Ra 509	Ac 666																



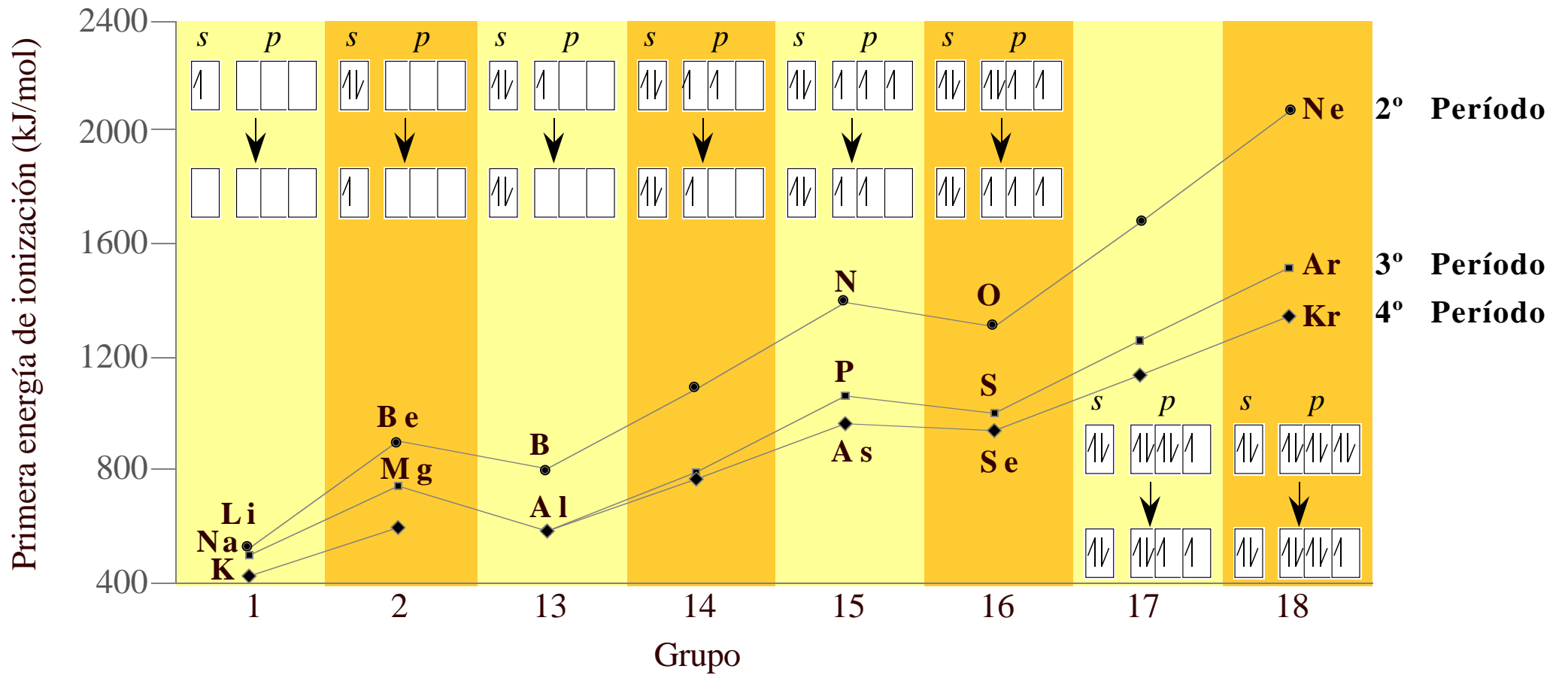
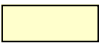

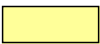





Tabla 1.14. Energías de ionización de los elementos del 2 al 5

Elemento	Primera	Segunda	Tercera	Cuarta
He	2372 kJ mol ⁻¹			
Li	519 kJ mol ⁻¹	7300 kJ mol ⁻¹		
Be	900 kJ mol ⁻¹	1760 kJ mol ⁻¹	14800 kJ mol ⁻¹	
B	799 kJ mol ⁻¹	2420 kJ mol ⁻¹	3660 kJ mol ⁻¹	25000 kJ mol ⁻¹

1												18									
H 72																He -21					
Li 60	Be -241															B 27	C 122	N 0	O 141	F 328	Ne -29
Na 53	Mg -230															Al 42	Si 134	P 72	S 200	Cl 349	Ar -34
K 48	Ca -156															Ga 29	Ge 119	As 78	Se 195	Br 325	Kr -39
Rb 47	Sr -167															In 29	Sn 107	Sb 103	Te 190	I 295	Xe -40
Cs 45	Ba -52															Tl 19	Pb 35	Bi 91	Po 183	At 270	Rn -41
Fr	Ra																				

 < 100	 +100 a +200
 -100 a 0	 +200 a +300
 0 a +100	 > +300