

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

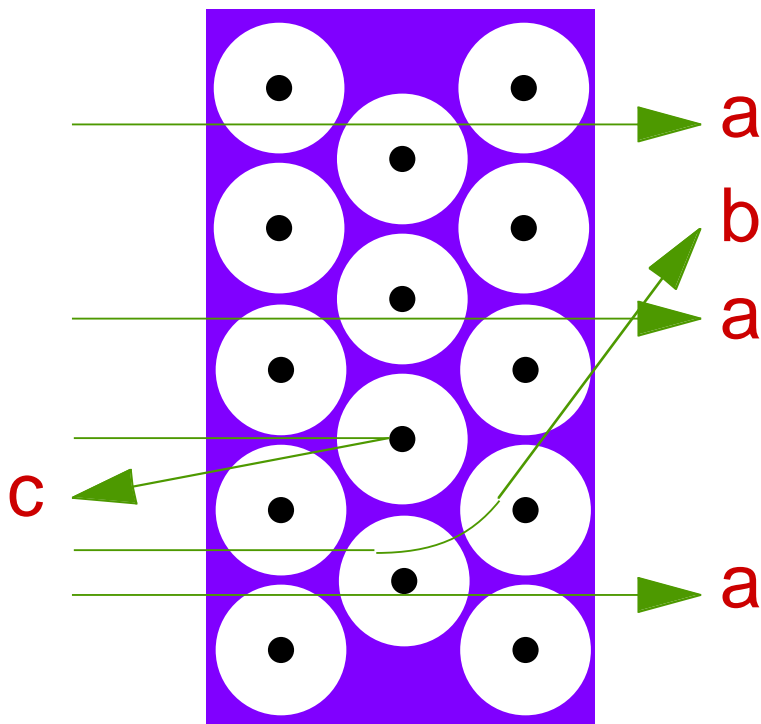
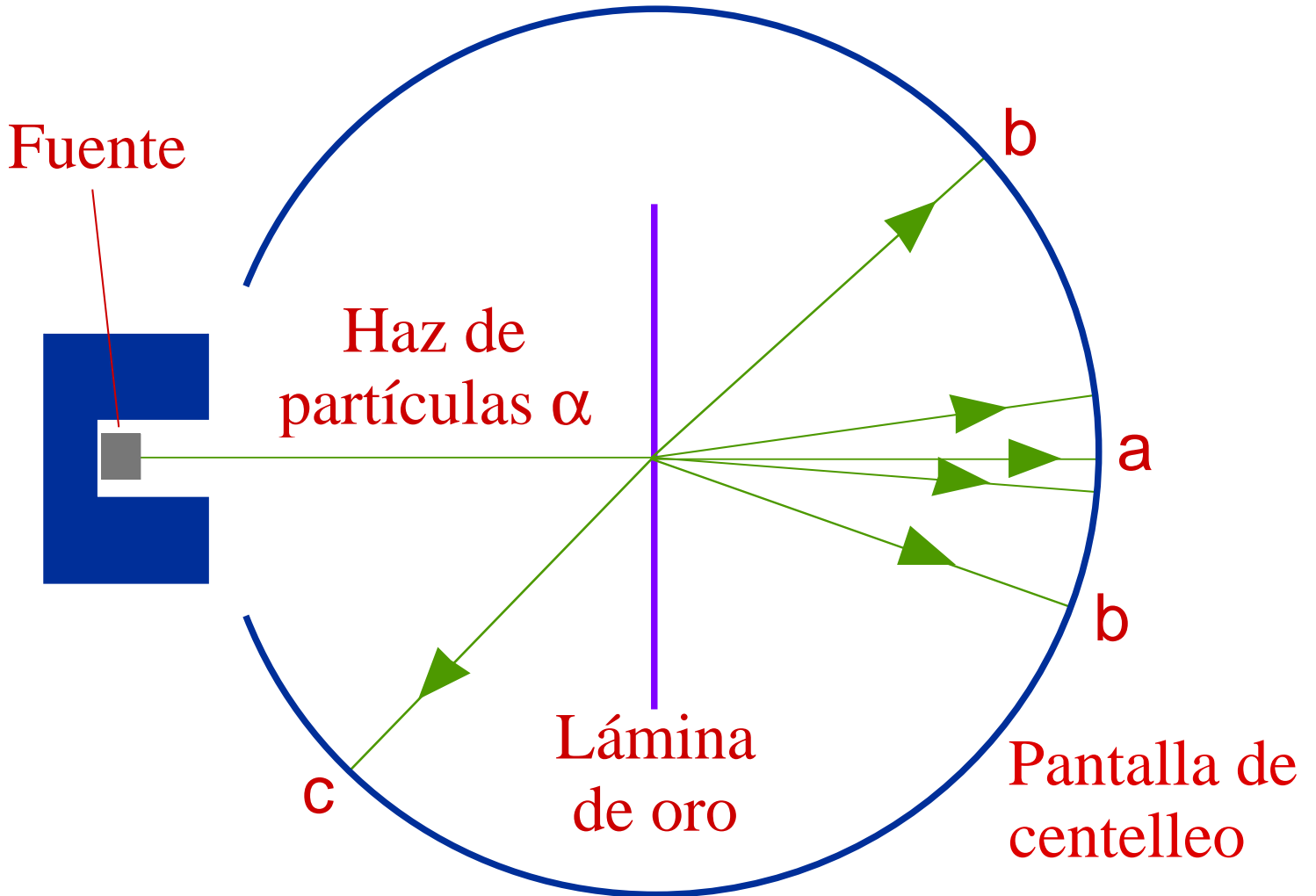
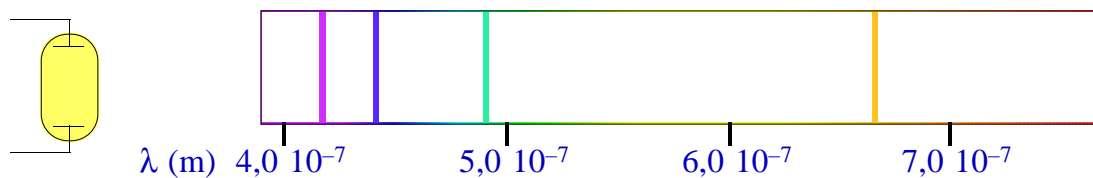
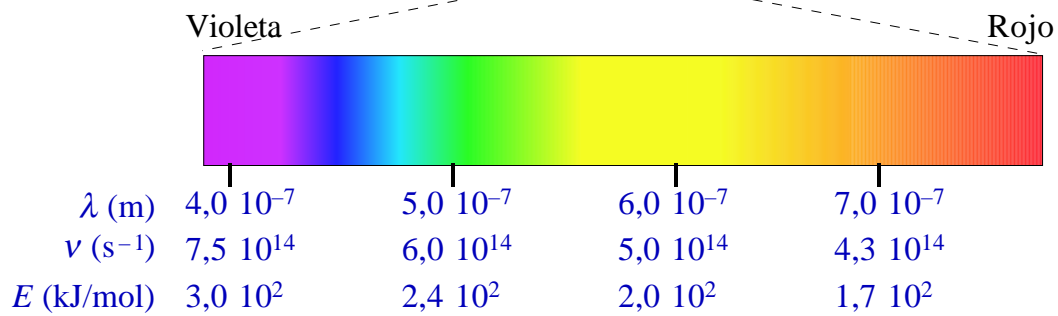
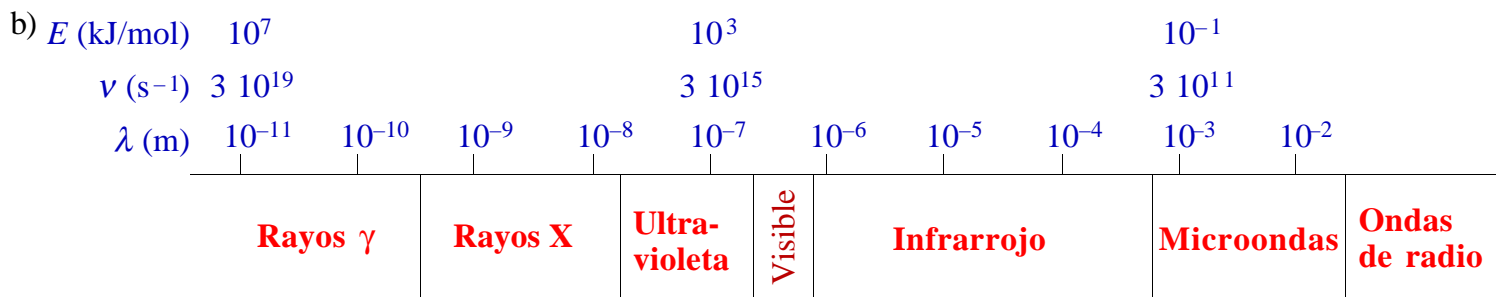
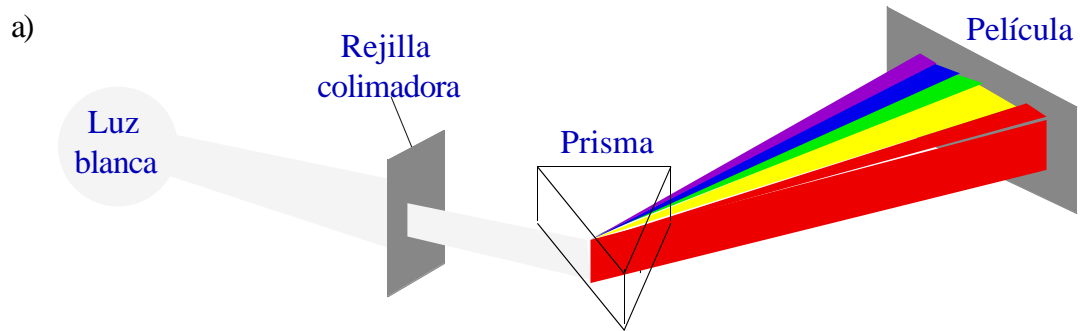
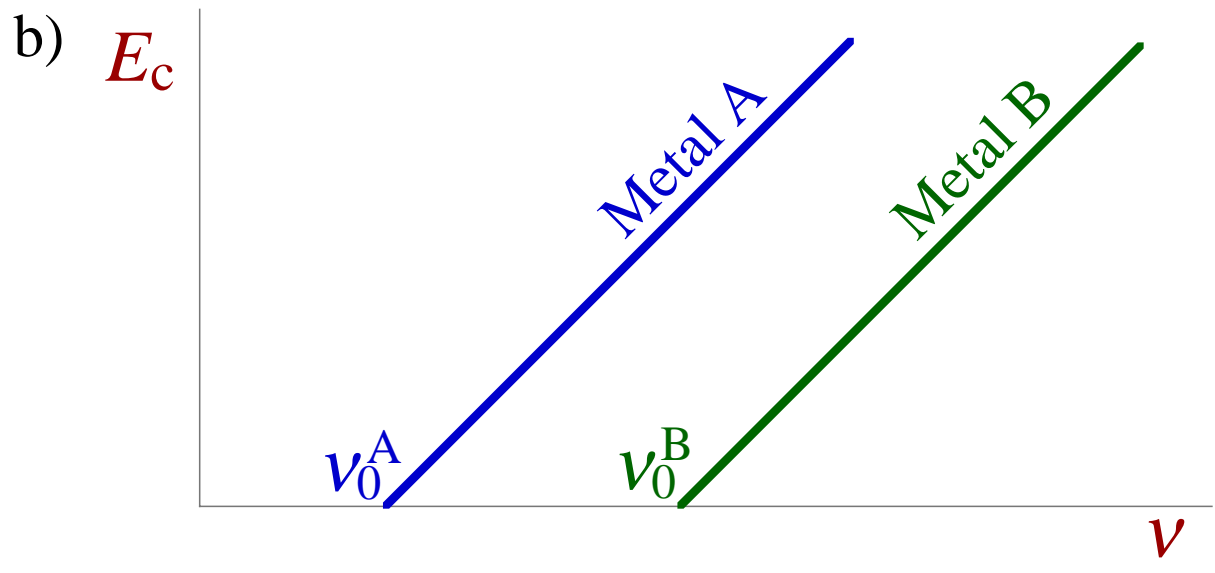
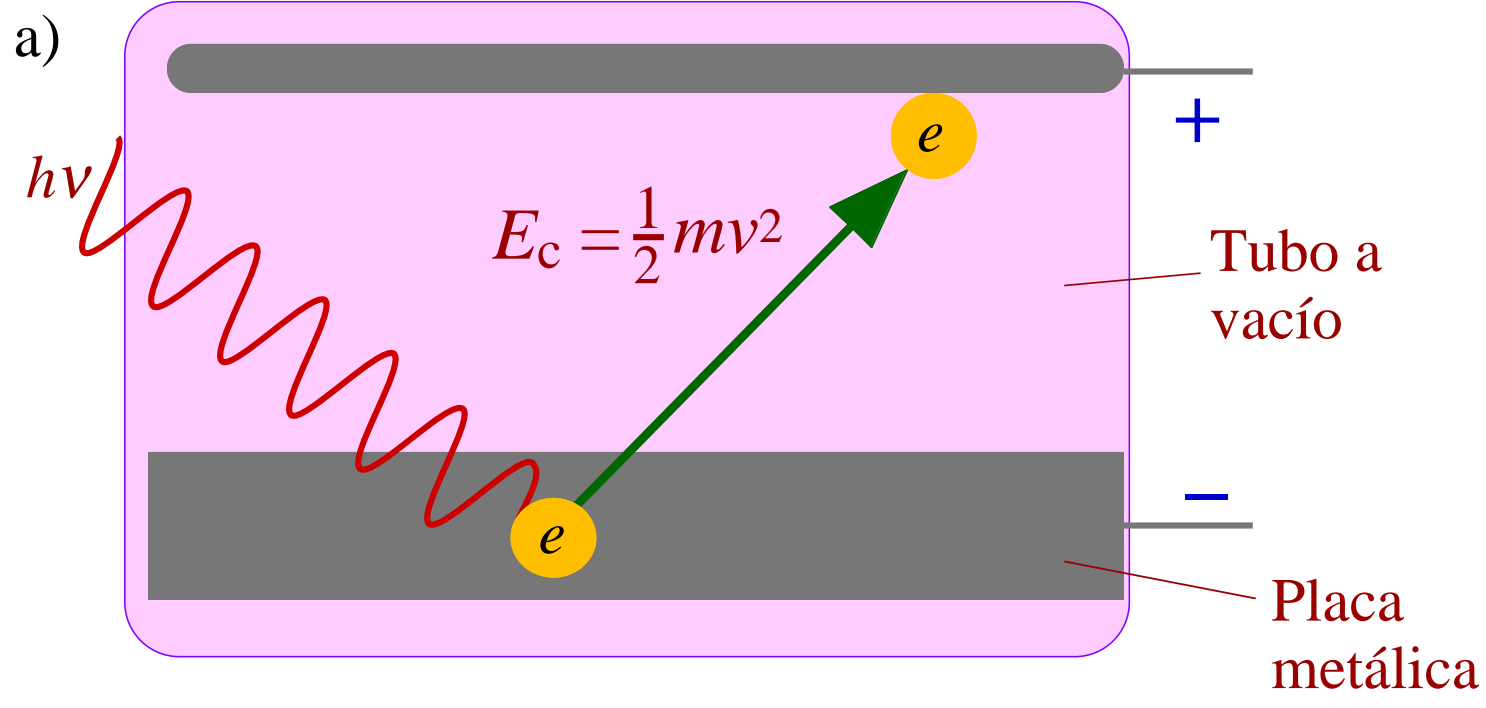
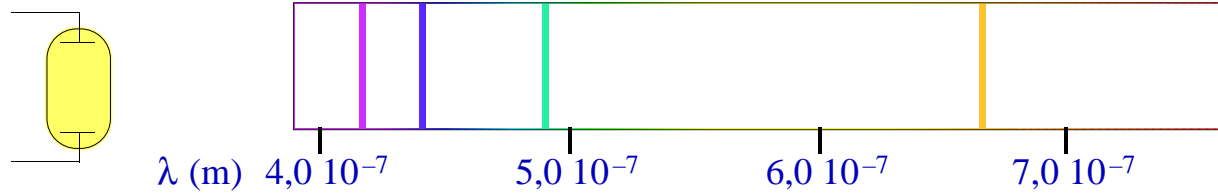


Tabla 1.2. Algunos elementos con varios isótopos

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



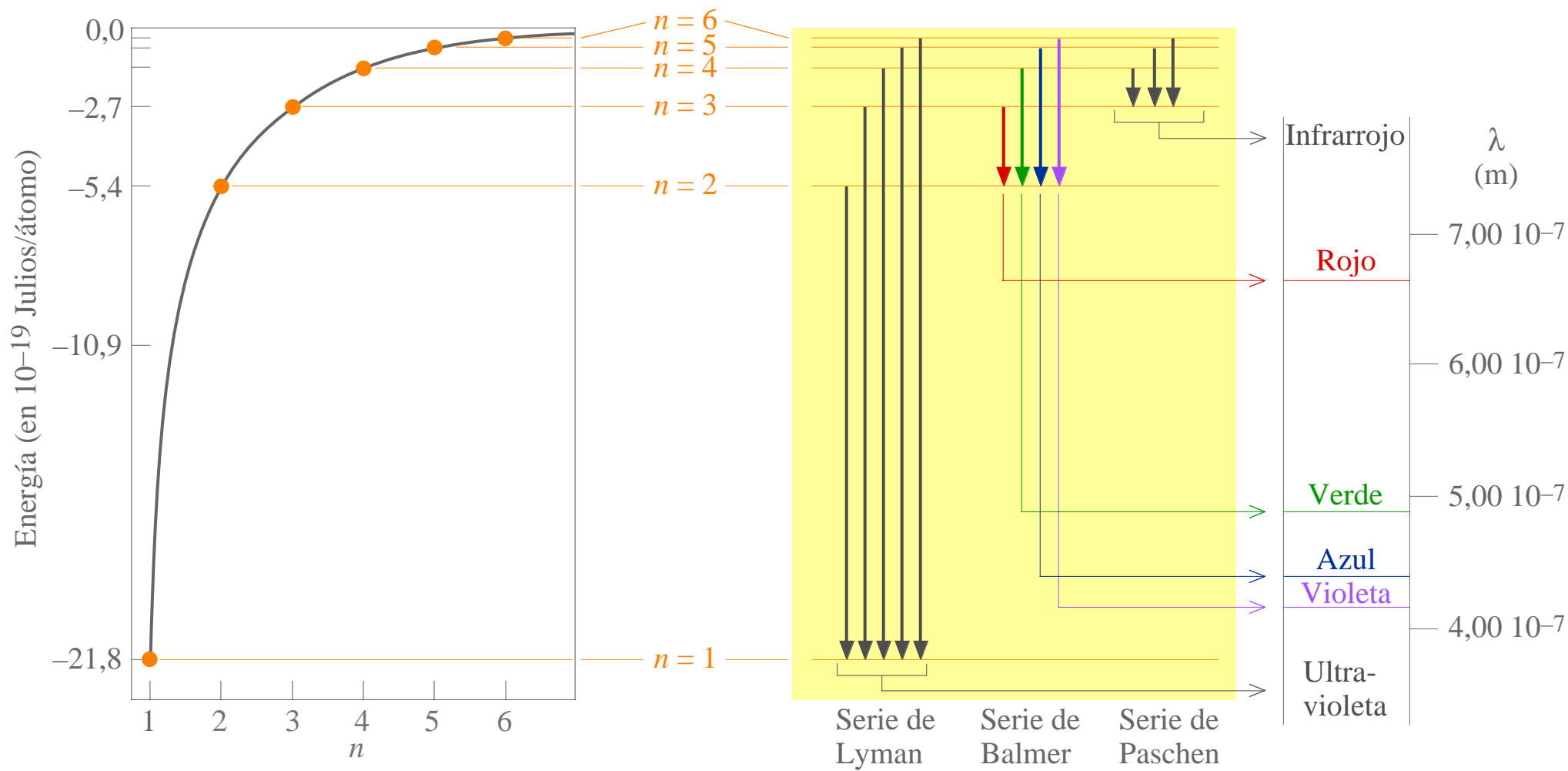




$$\nu = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

$R_H = 3,29 \cdot 10^{15} \text{ s}^{-1}$ (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	$n_1 = 3$	$n_2 = 4, 5, 6, 7 \dots$			



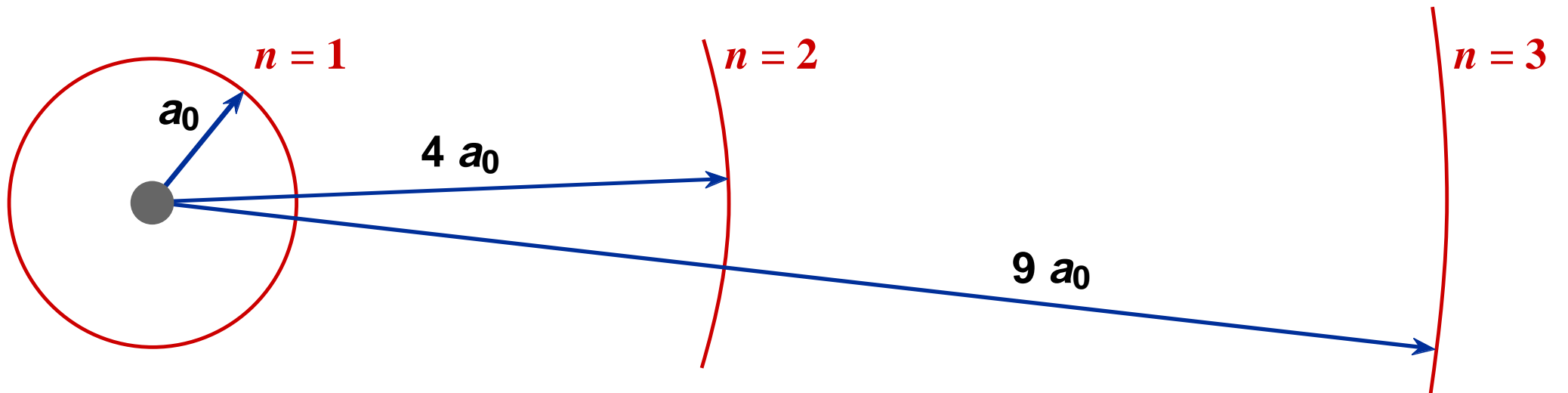


Tabla 1.3. Números cuánticos del átomo de hidrógeno

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

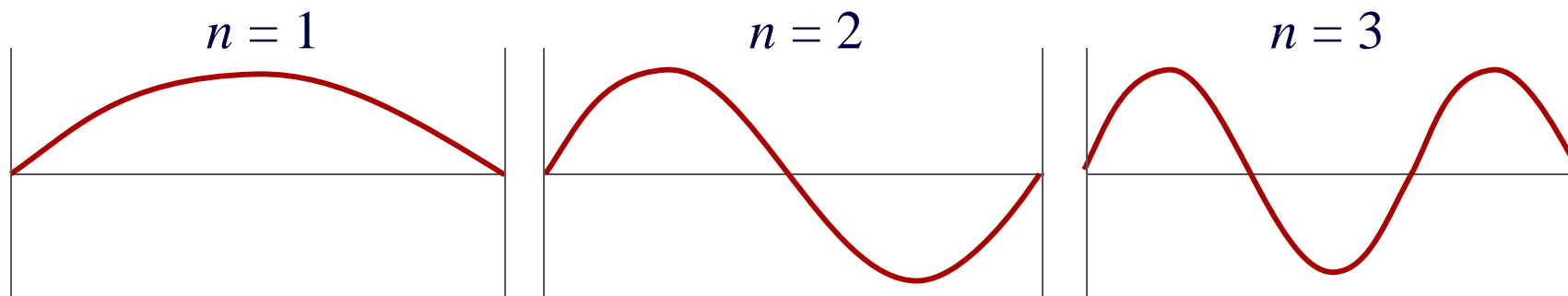
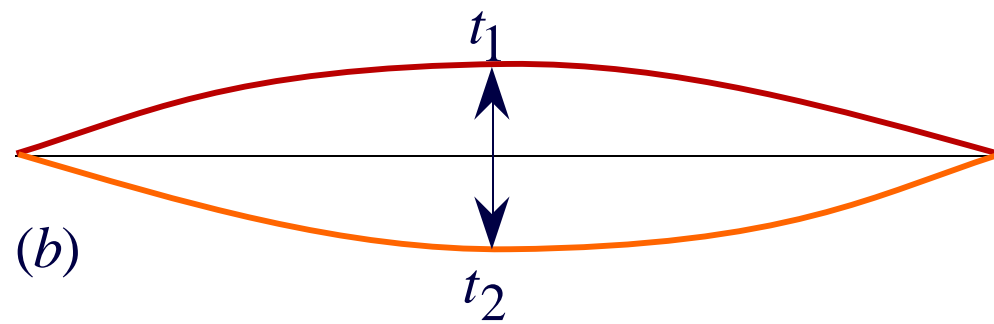
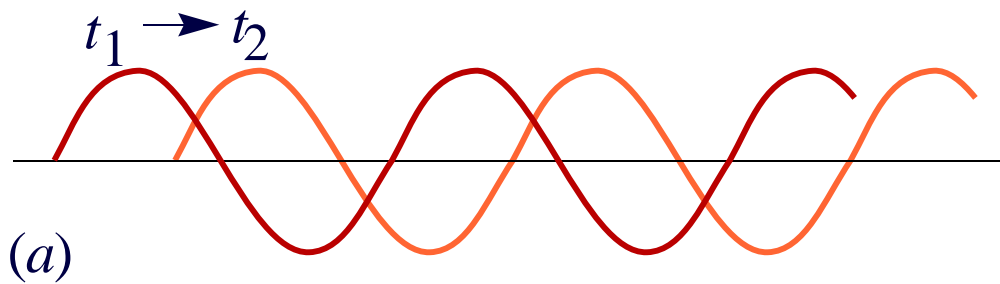
*También llamado momento angular orbital; ***órbita* en el lenguaje de Bohr, *orbital* en el de la mecánica cuántica.

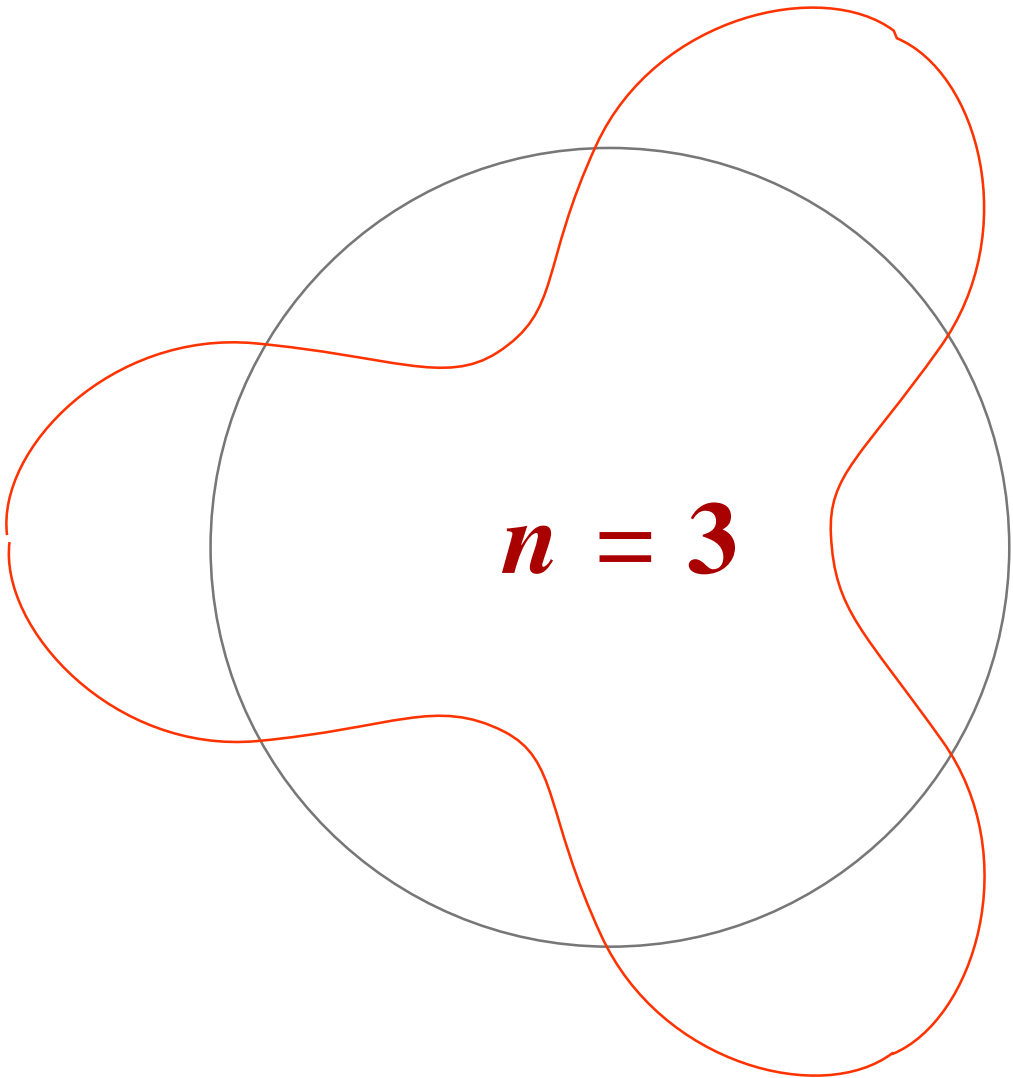
Tabla 1.4. Longitudes de onda de partículas

Partícula	Masa (kg)	Velocidad ($m s^{-1}$)	Longitud de onda (Å)
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	$3,3 \cdot 10^{-24}$

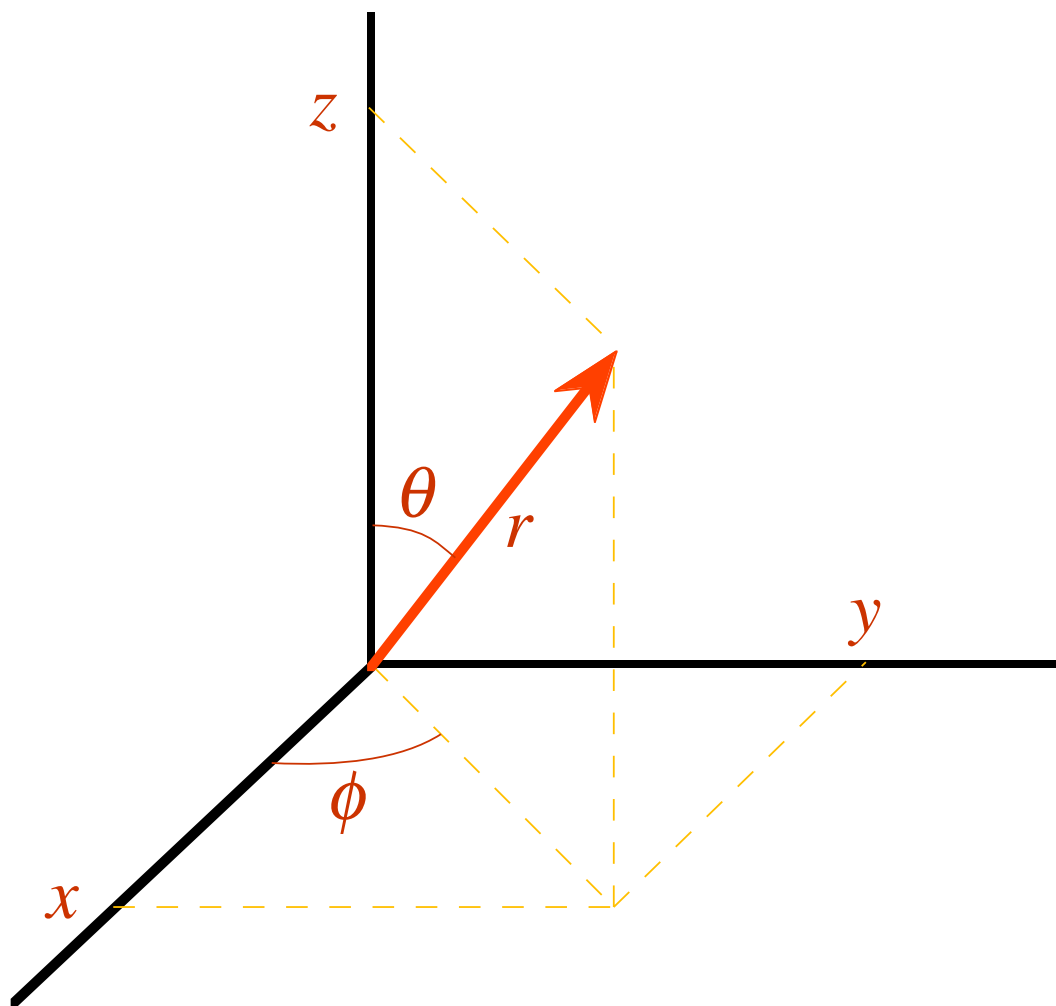
Ejemplo. Imprecisión mínima en la posición de partículas cuya imprecisión en la velocidad es del 1%

<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

$$z = r \cos \theta$$

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

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

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

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

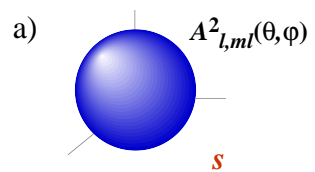
$$\phi = \arctg(y/x)$$

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

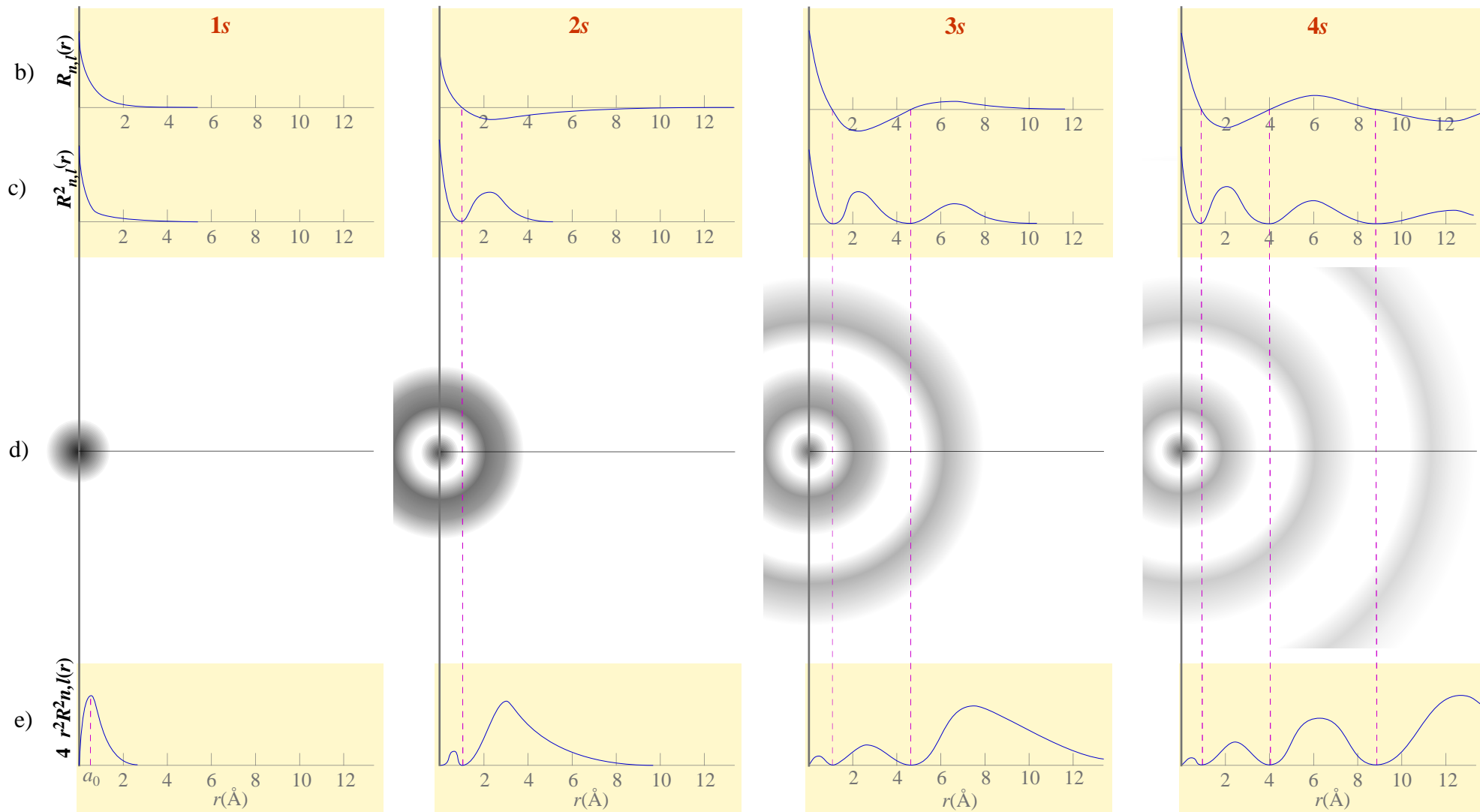
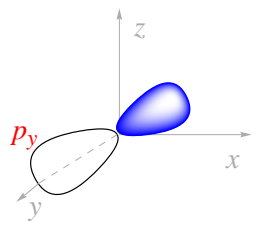
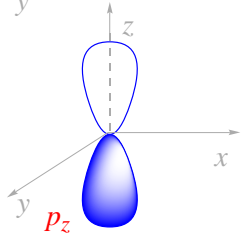
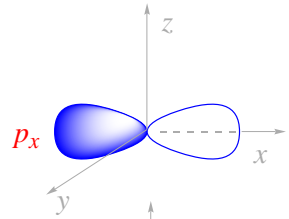


Tabla 1.7. Funciones angulares A_{l,m_l} normalizadas para átomos o iones monoelectrónicos

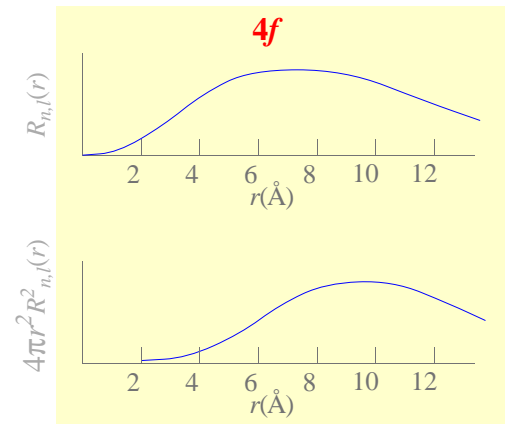
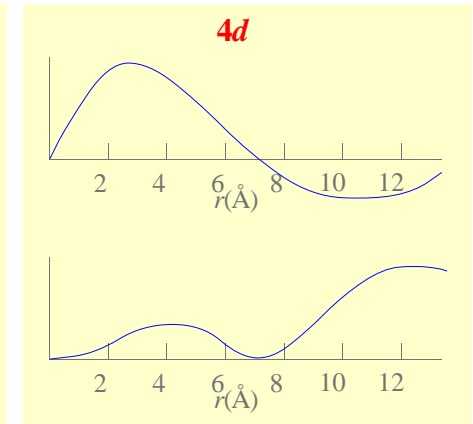
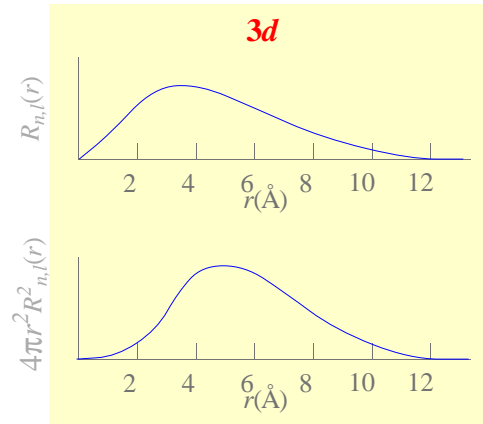
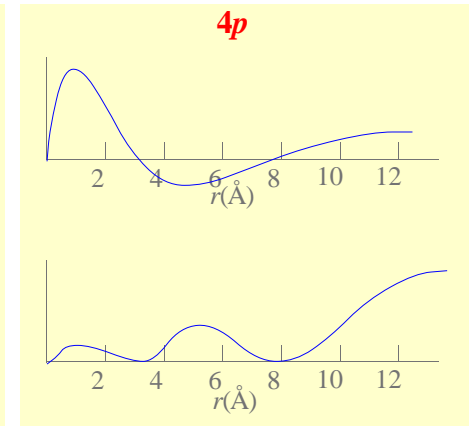
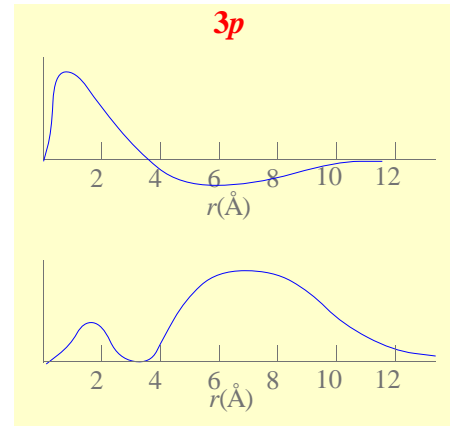
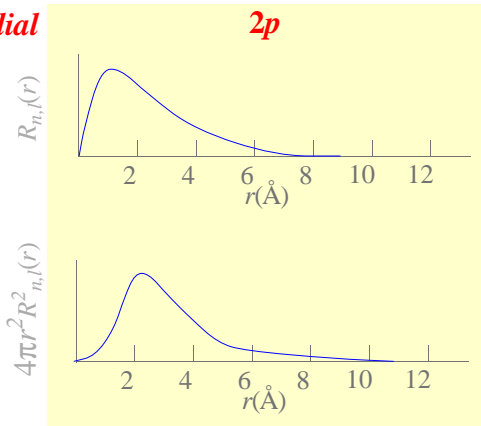
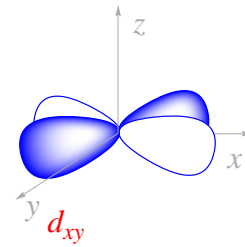
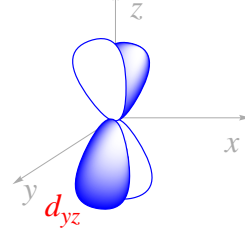
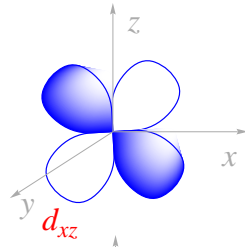
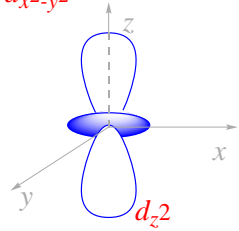
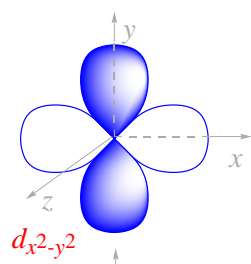
Orbital	$A_{l,m_l}(\theta, \phi)^*$	$A_{l,m_l}(x, y, z)^{**}$
s	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
p_z	$\frac{\sqrt{3}}{2\sqrt{\pi}} \cos \theta$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (z/r)$
p_x	$\frac{\sqrt{3}}{2\sqrt{\pi}} \text{sen } \theta \cos \phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (x/r)$
p_y	$\frac{\sqrt{3}}{2\sqrt{\pi}} \text{sen } \theta \text{sen } \phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (y/r)$
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}	$\frac{\sqrt{70}}{8\sqrt{\pi}} \text{sen}^3 \theta (3 \text{sen } \phi - 4 \text{sen}^3 \phi)$	$\frac{\sqrt{70}}{8\sqrt{\pi}} [(-y^3 + 3x^2y)/r^3]$

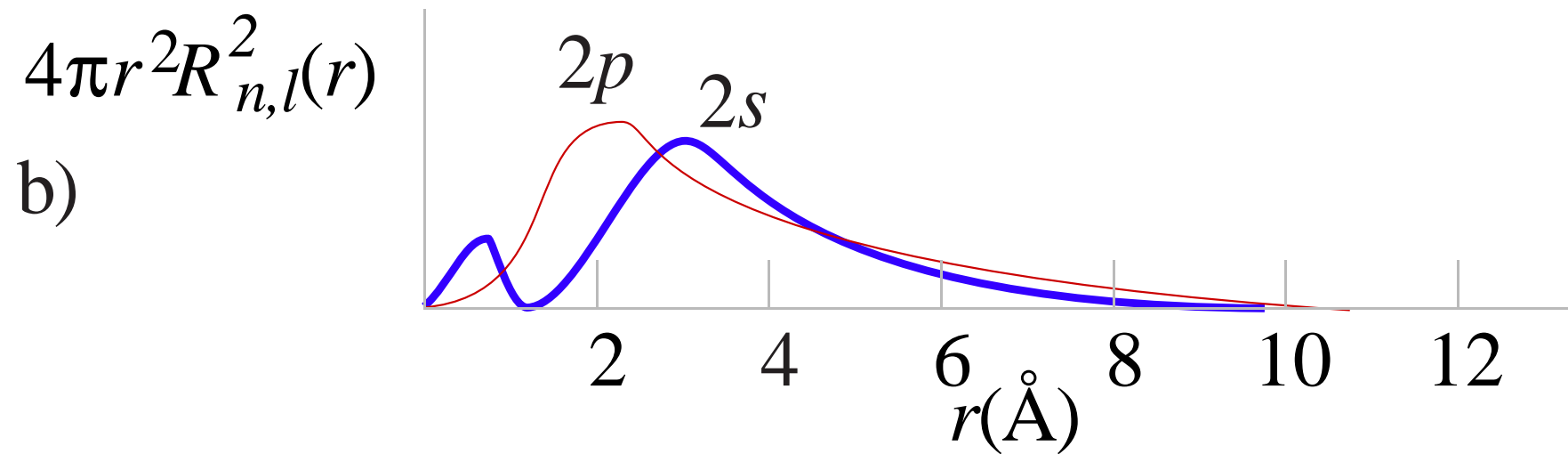
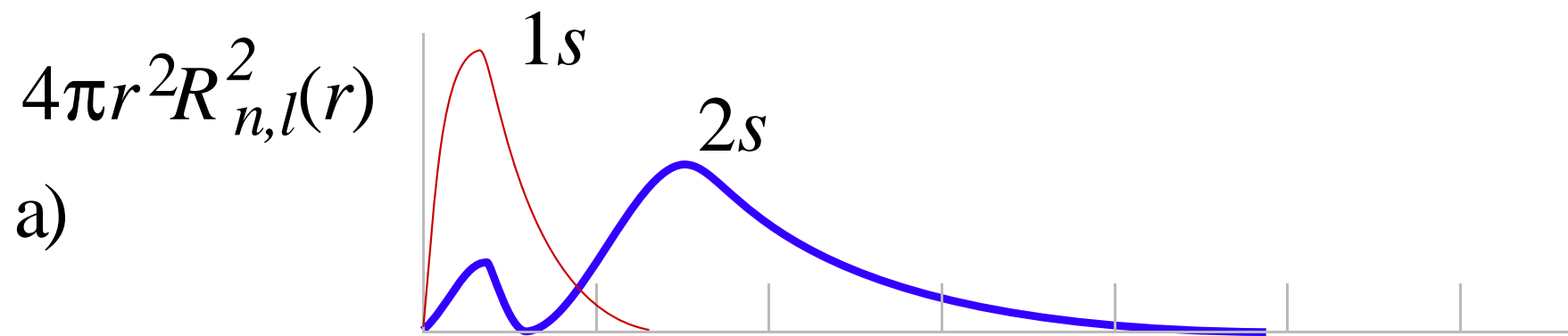
* Funciones en el sistema de coordenadas polares esféricas. ** Funciones en el sistema de coordenadas cartesiano.

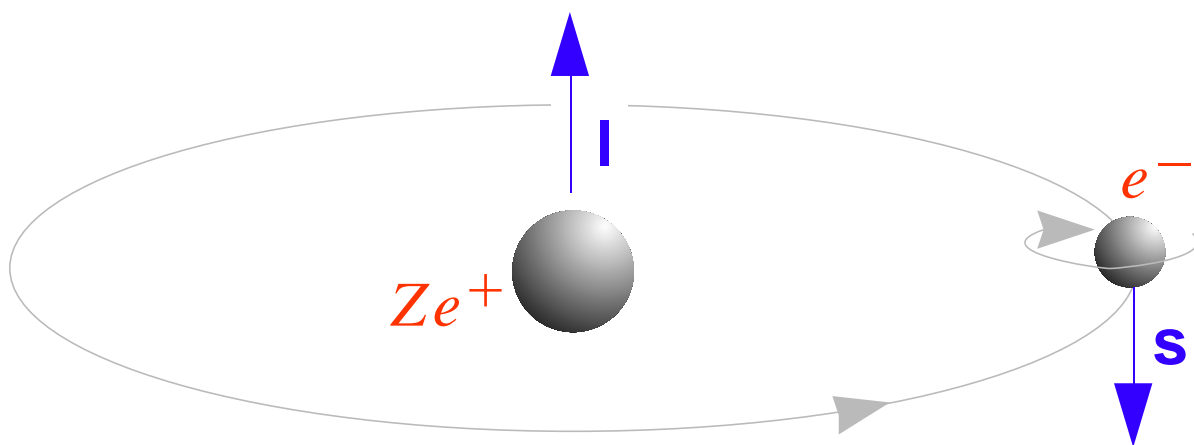
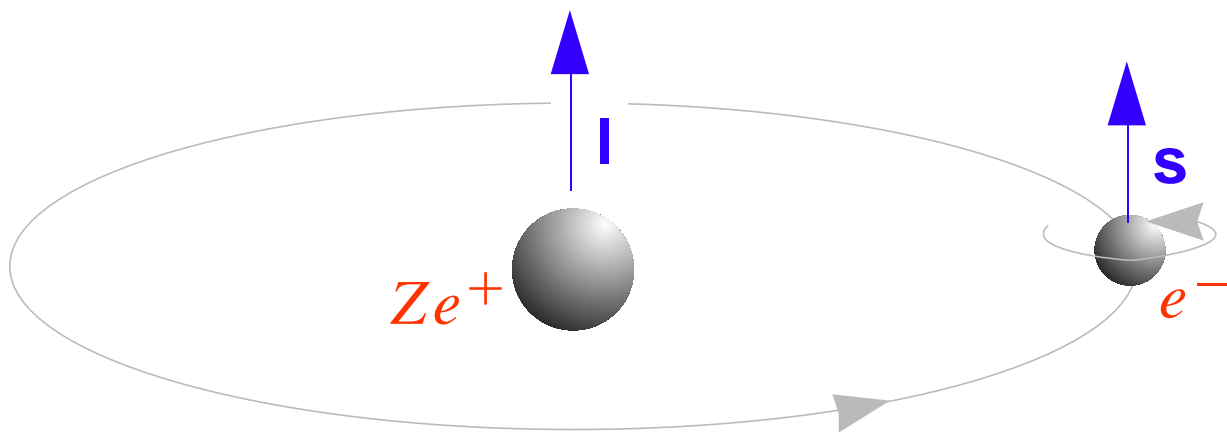
Parte Angular



Parte Radial







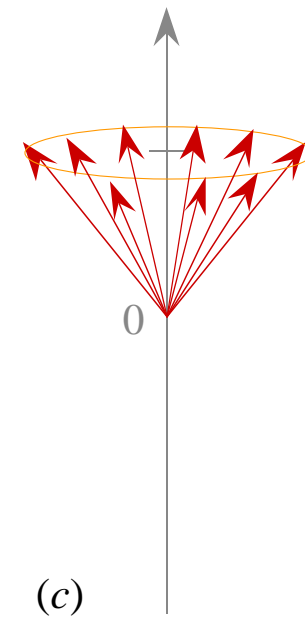
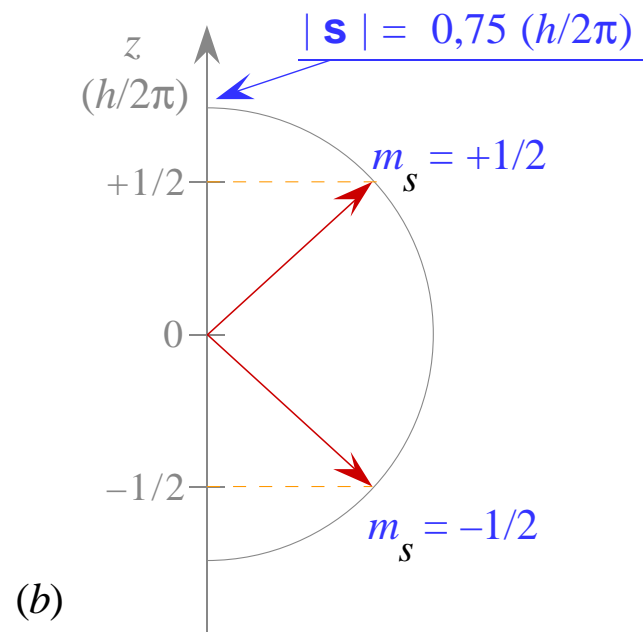
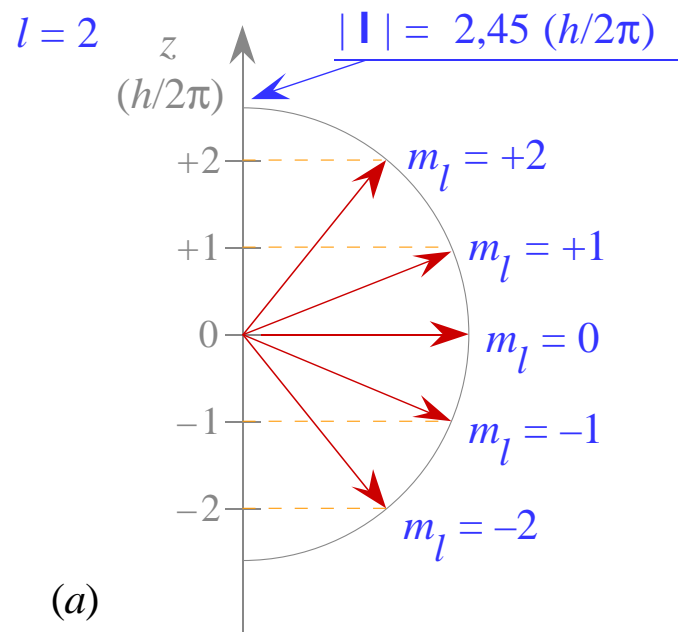
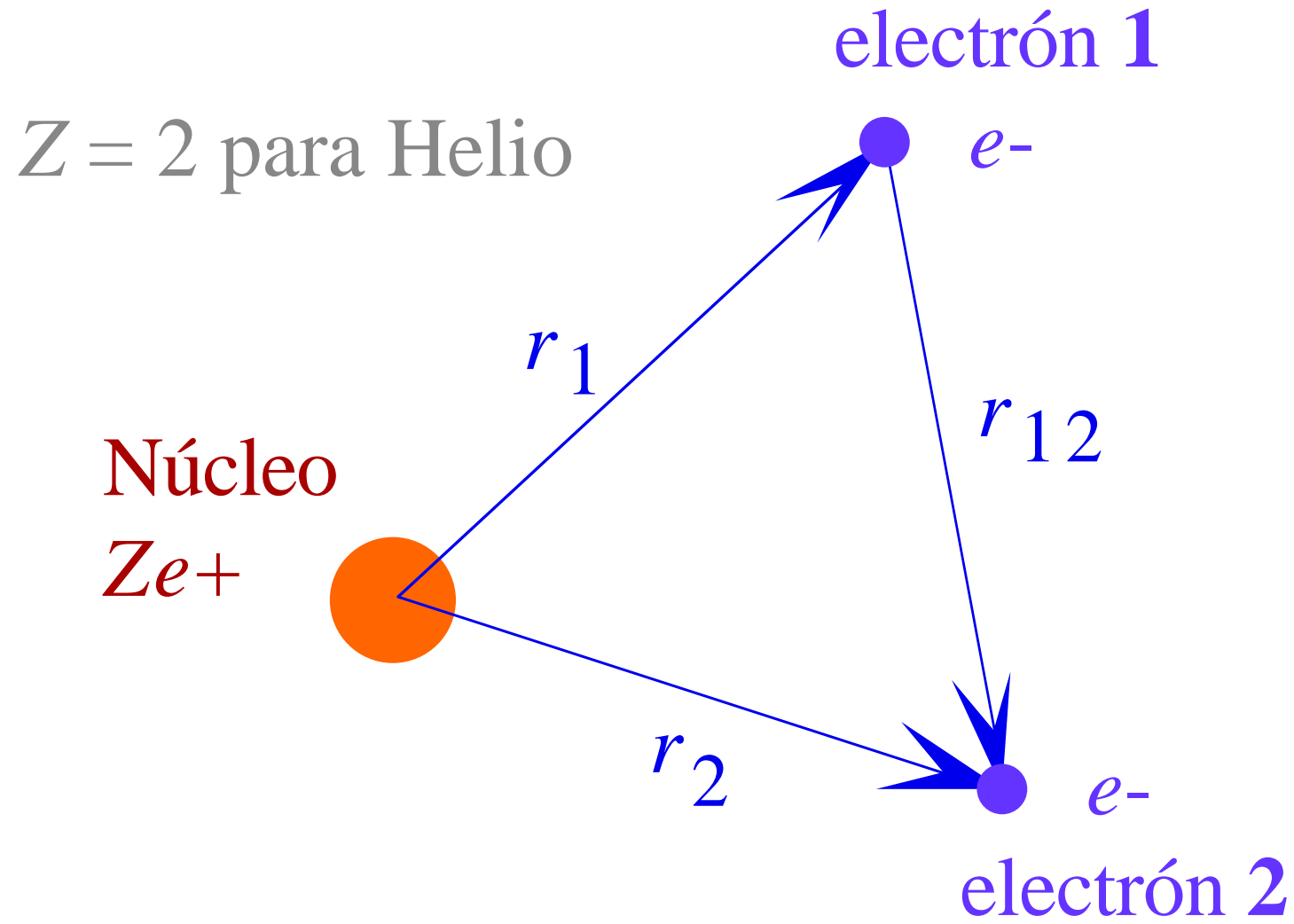


Tabla 1.8. Niveles de energía de un electrón en un orbital del hidrógeno, considerando la interacción espín-órbita

<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



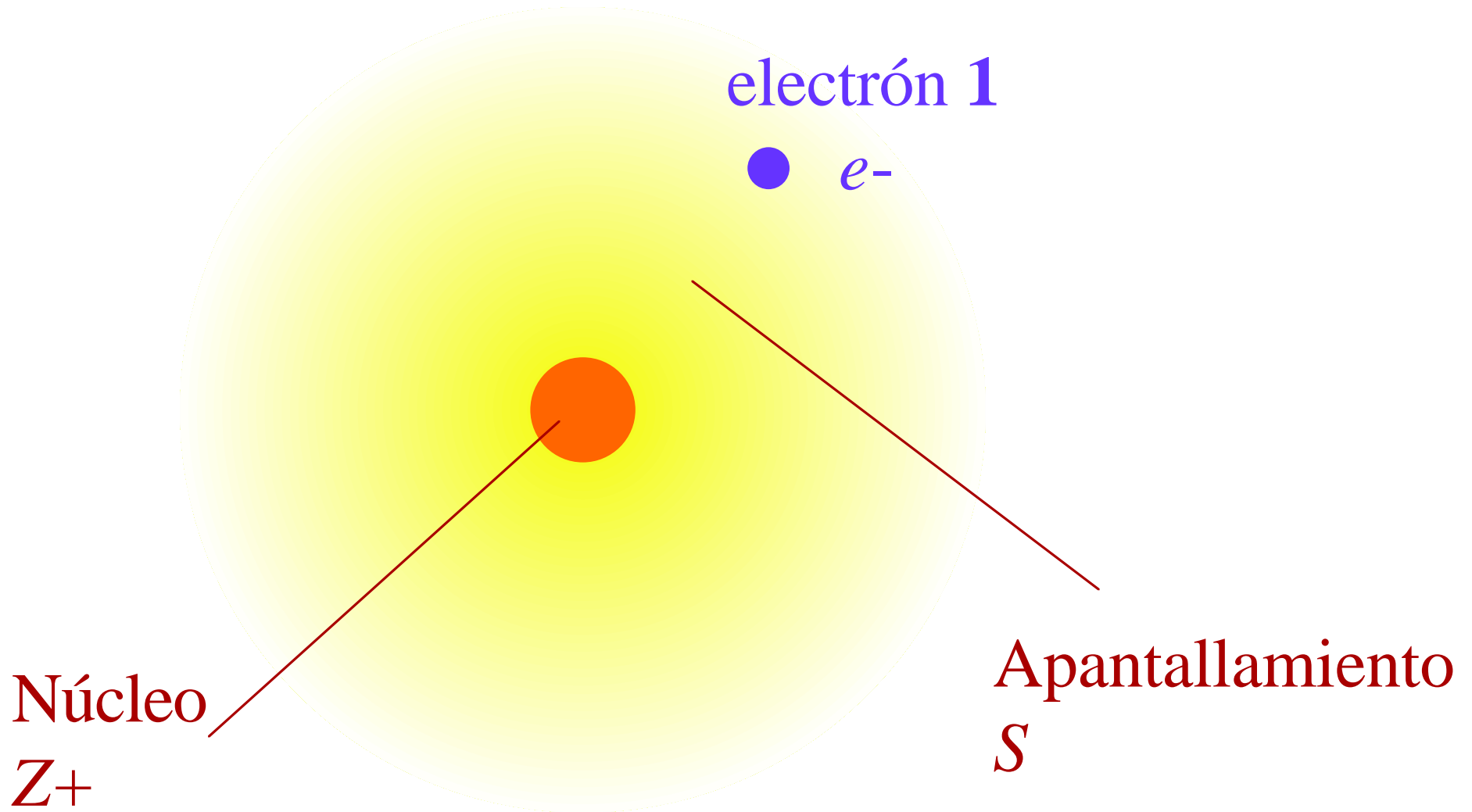
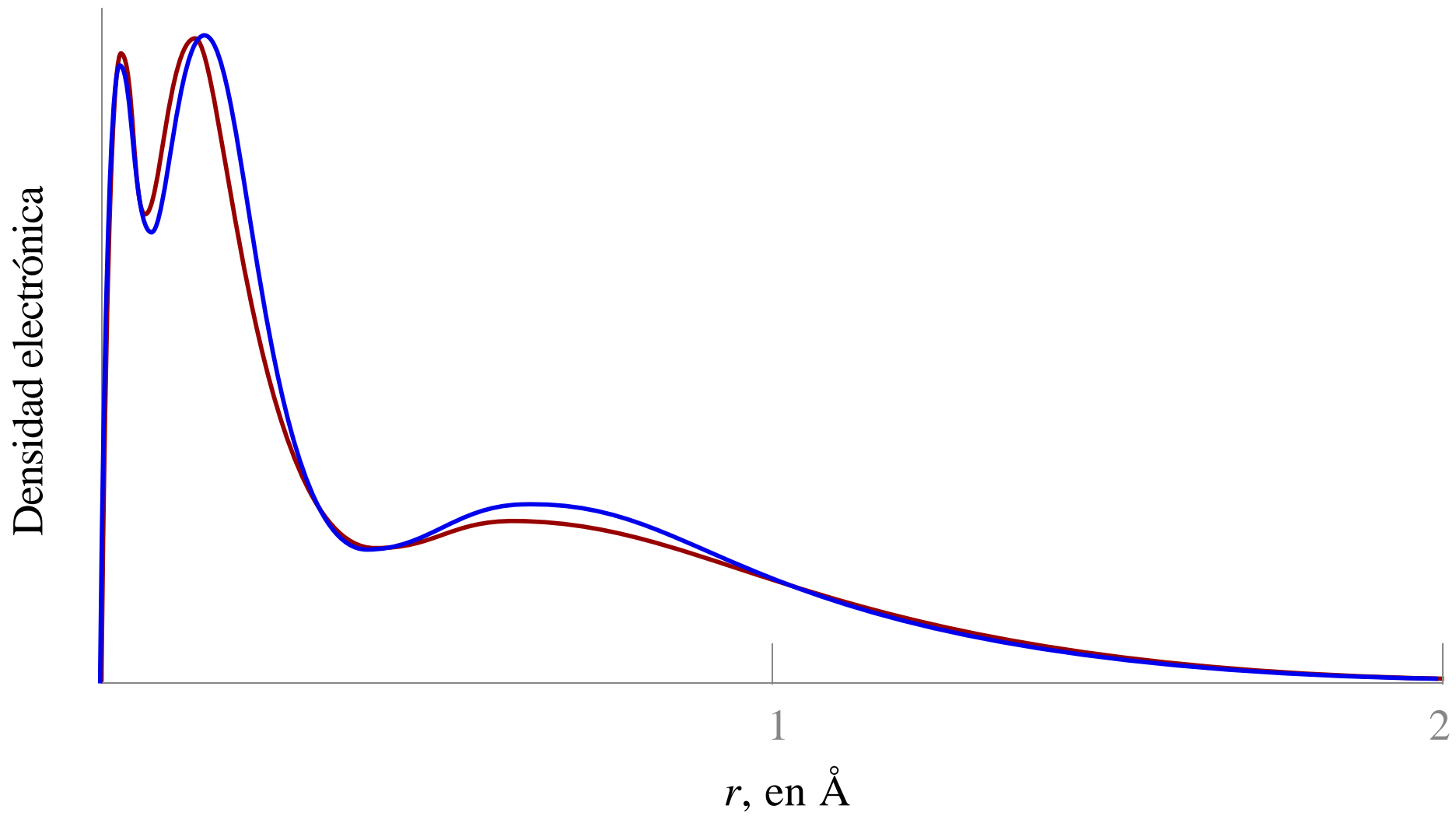


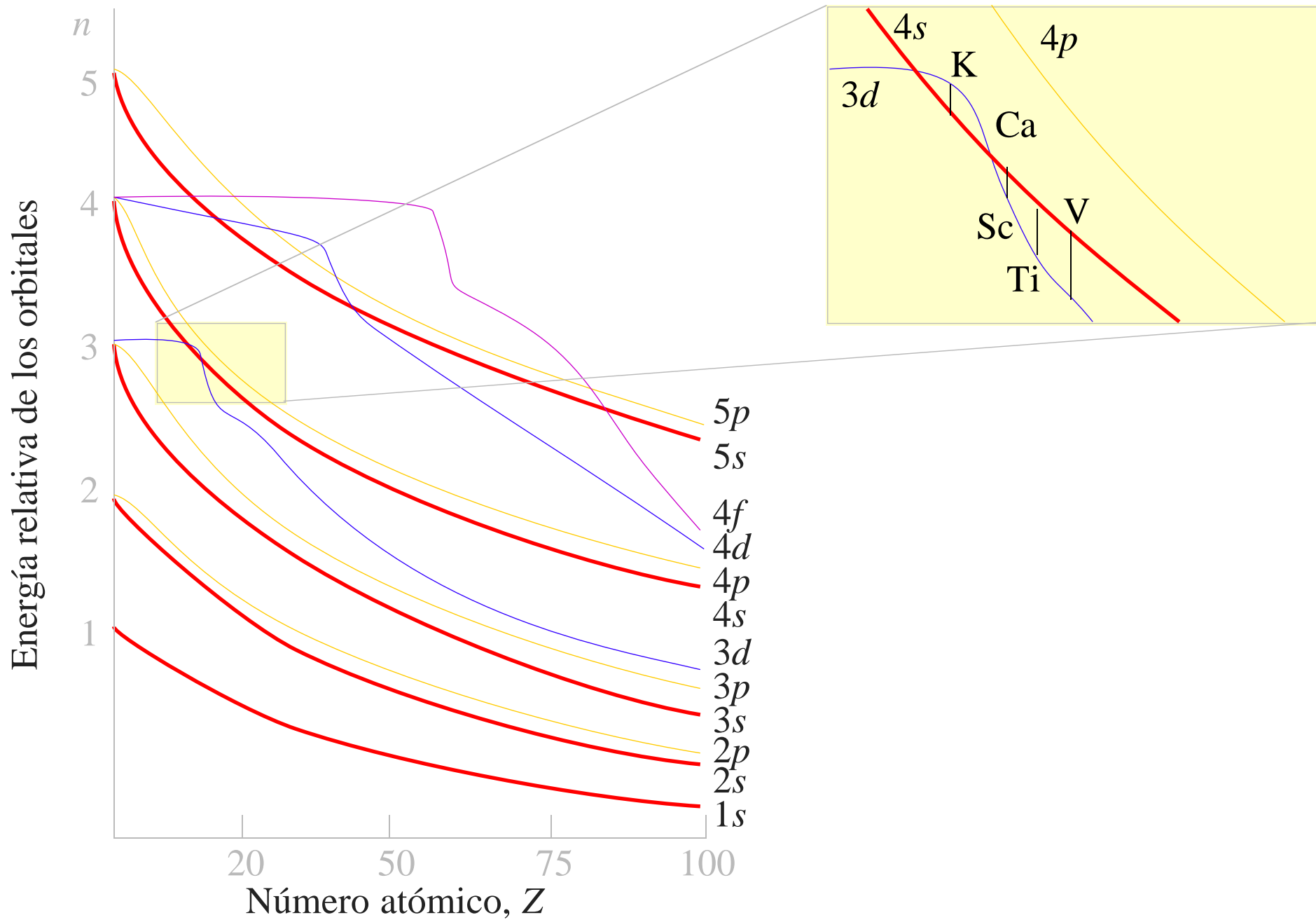
Tabla 1.9 (parcial). Cargas Nucleares Efectivas de los elementos del 1 al 36

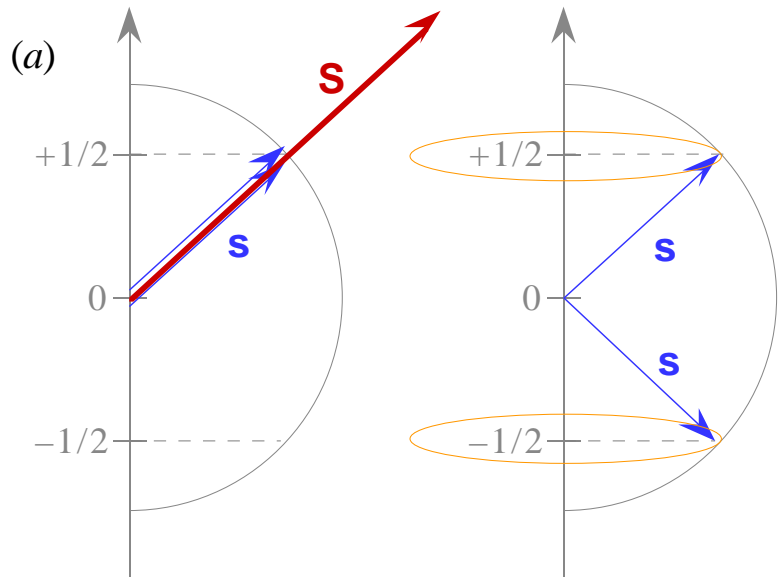
Elemento	1s	2s	2p	3s	3p	4s
H	1,000					
He	1,688					
Li	2,691	1,279				
Be	3,685	1,912				
B	4,680	2,576	2,421			
C	5,673	3,217	3,136			
N	6,665	3,847	3,834			
O	7,658	4,492	4,453			
F	8,650	5,128	5,100			
Ne	9,642	5,758	5,758			
Na	10,626	6,571	6,802	2,507		
Mg	11,619	7,392	7,826	3,308		
Al	12,591	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

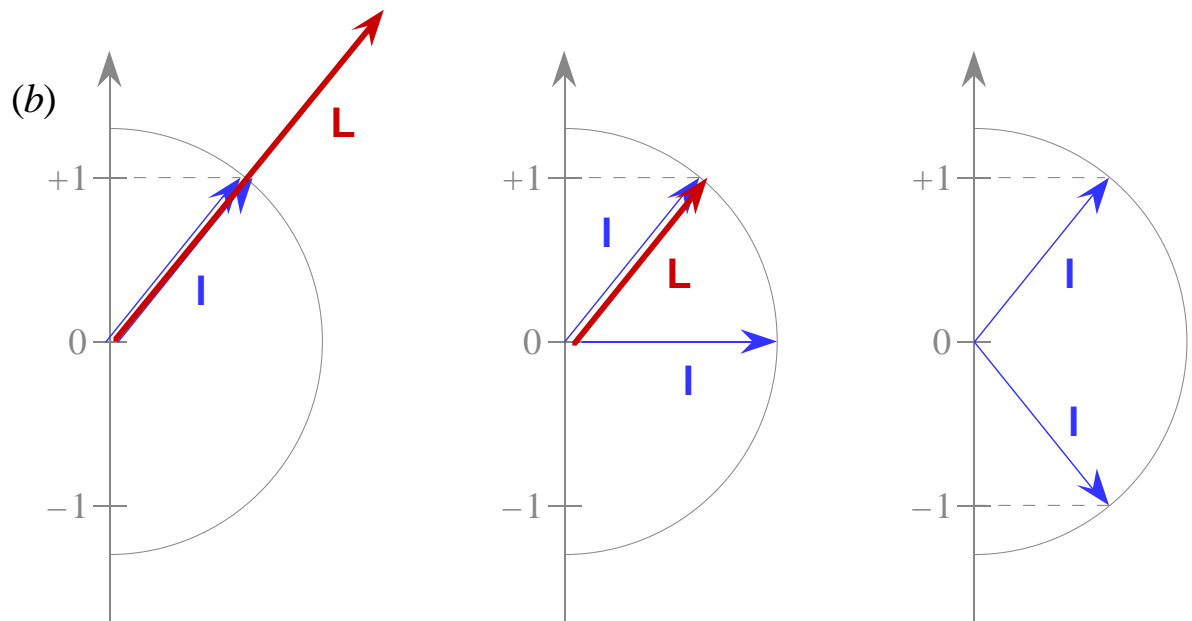






$s = 1/2$
 $S = 1$
 $M_S = +1, 0, -1$

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



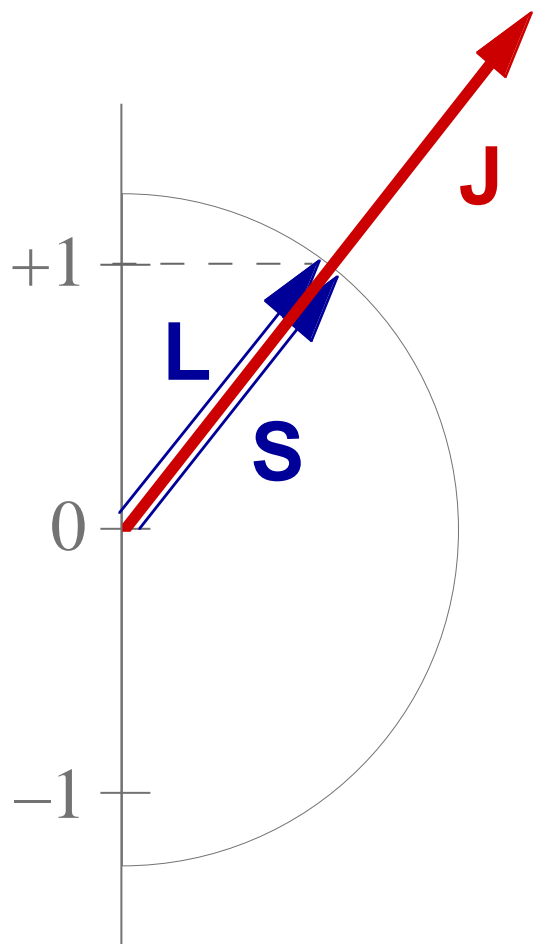
$l = 1$
 $L = 2$
 $M_L = +2, +1, 0, -1, -2$

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

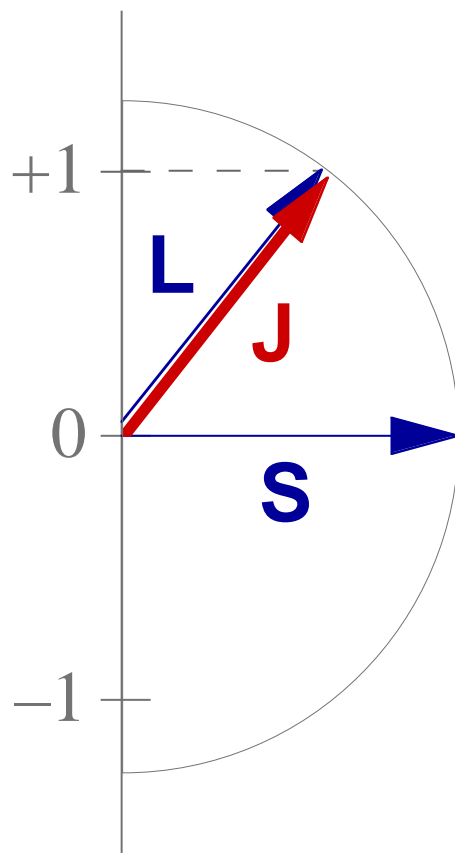
$l = 1$
 $L = 0$
 $M_L = 0$

Tabla 1.12. Términos Russell–Saunders para algunas configuraciones

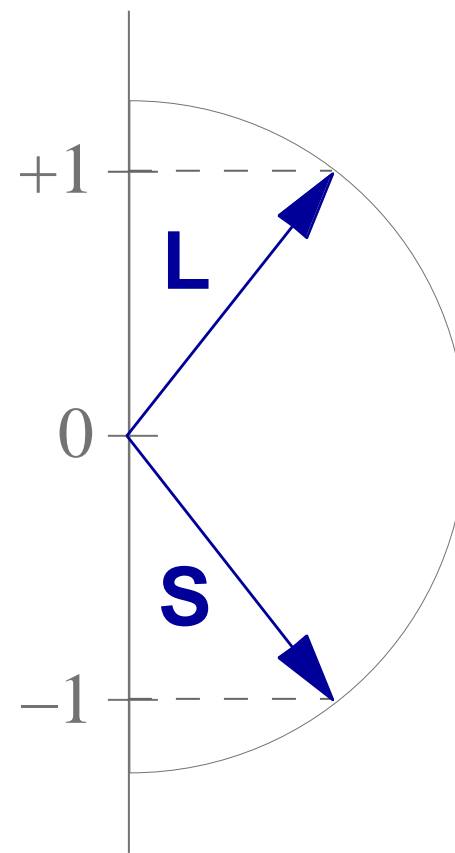
Configuración	Términos	Término fundamental
s^1	2S	2S
s^2	1S	1S
p^1 y p^5	2P	2P
p^2 y p^4	$^1S, ^1D, ^3P$	3P
p^3	$^2P, ^2D, ^4S$	4S
p^6	1S	1S
d^1 y d^9	2D	2D
d^2 y d^8	$^1S, ^1D, ^1G, ^3P, ^3F$	3F
d^3 y d^7	$^2P, ^2D(2), ^2F, ^2G, ^2H, ^4P, ^4F$	4F
d^4 y d^6	$^1S(2), ^1D(2), ^1F, ^1G(2), ^1I, ^3P(2),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



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



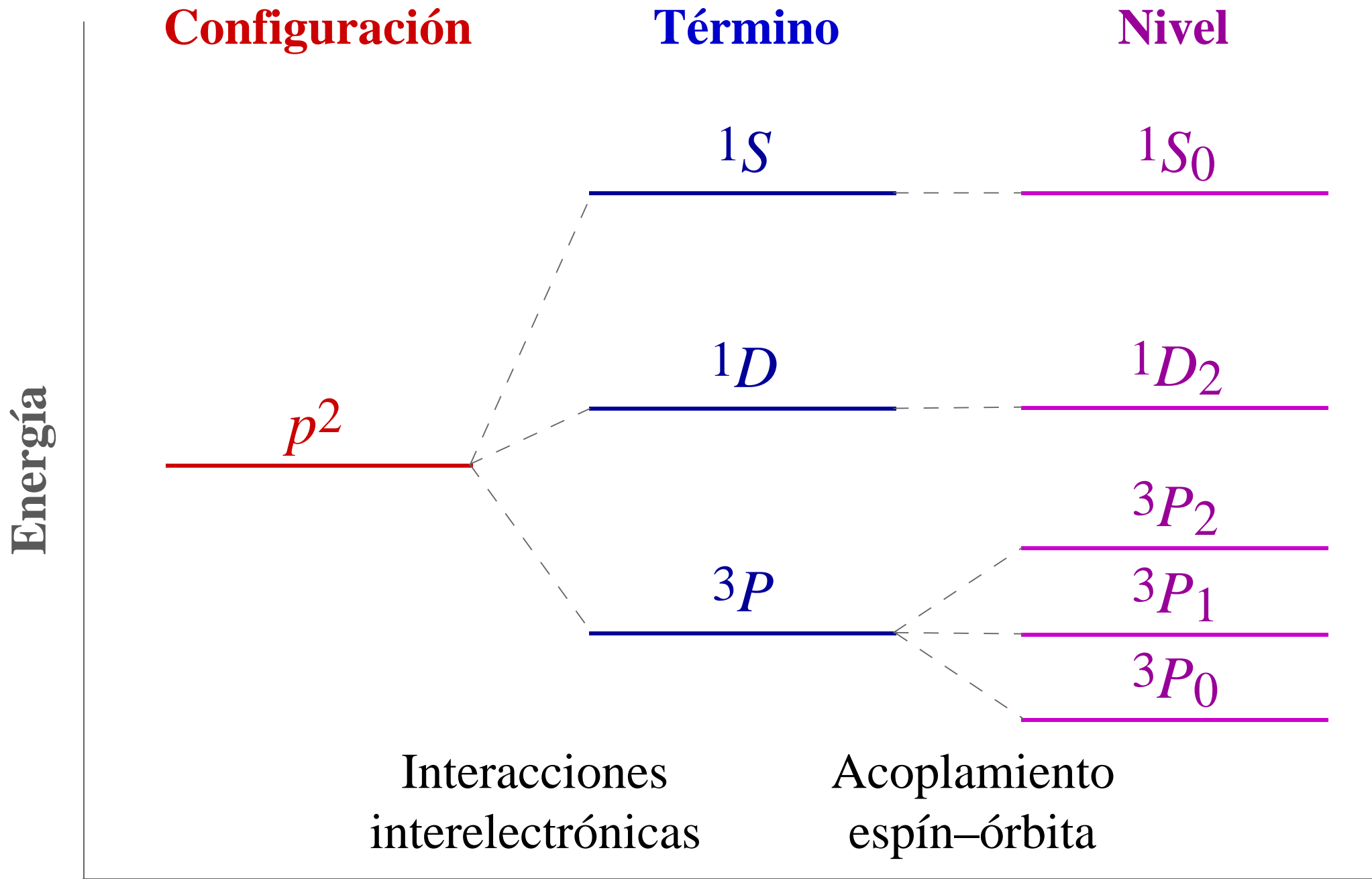
(b)
 $M_S = 0$
 $J = 1$

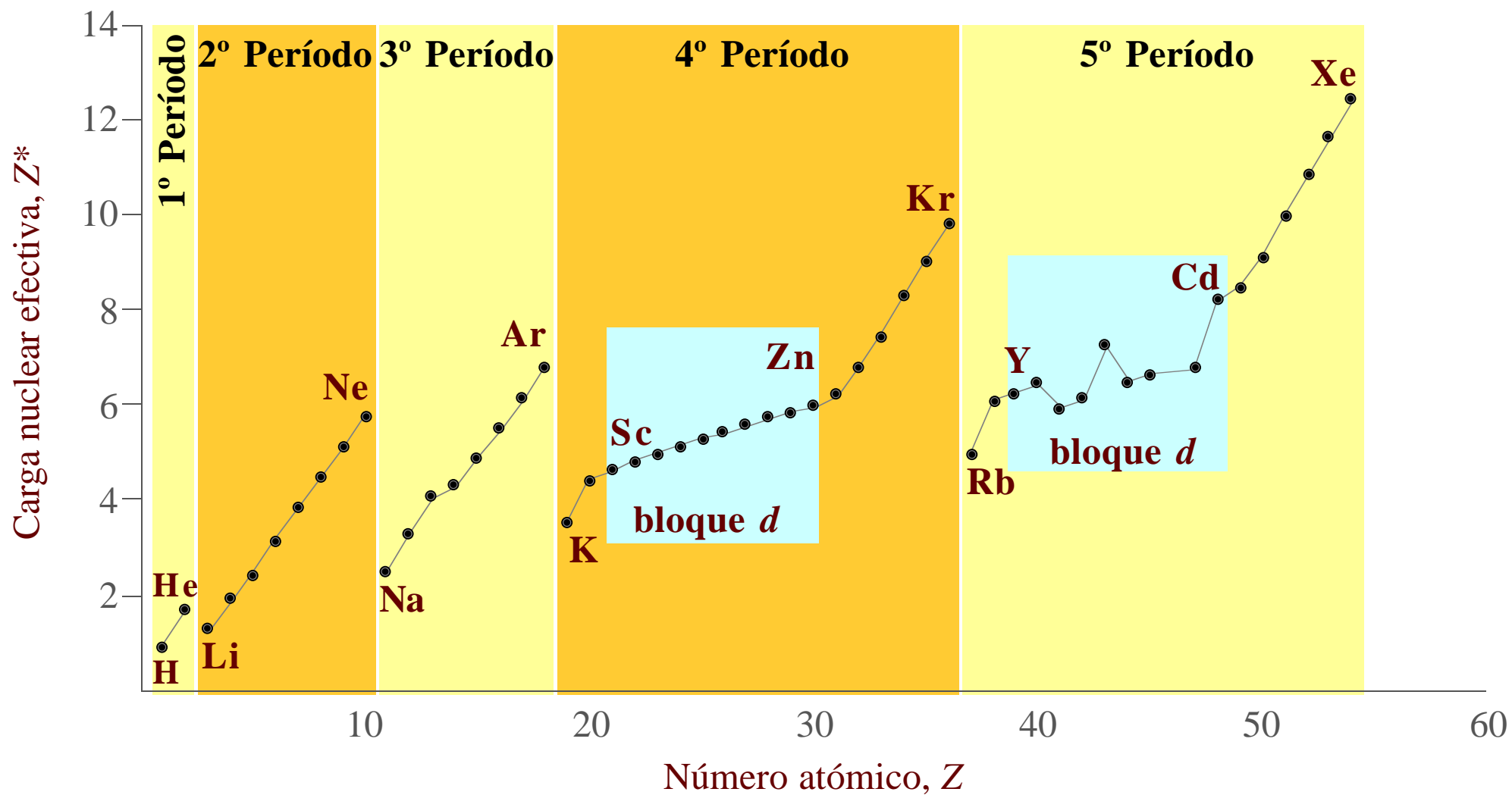


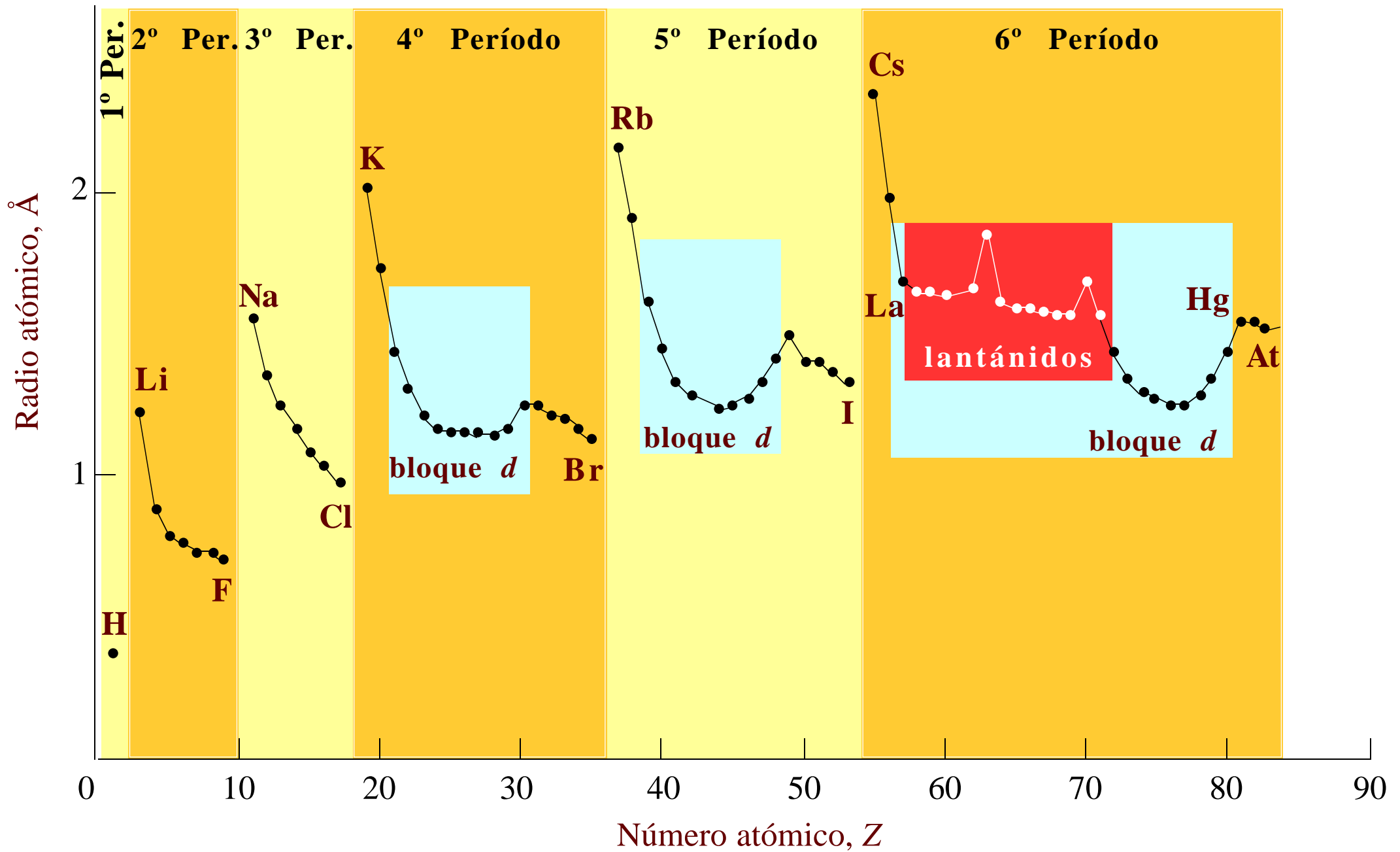
(c)
 $M_S = -1$
 $J = 0$

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

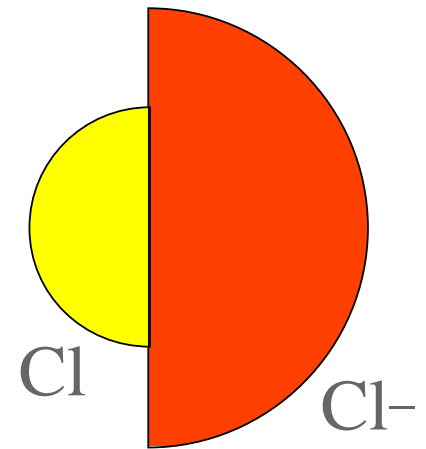
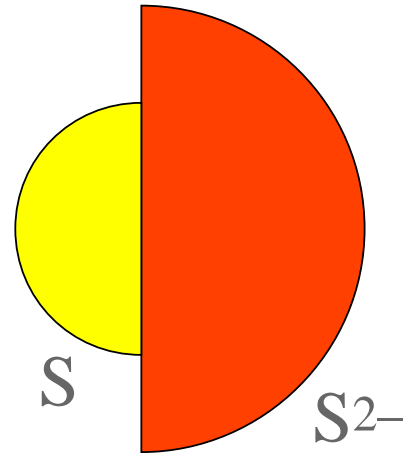
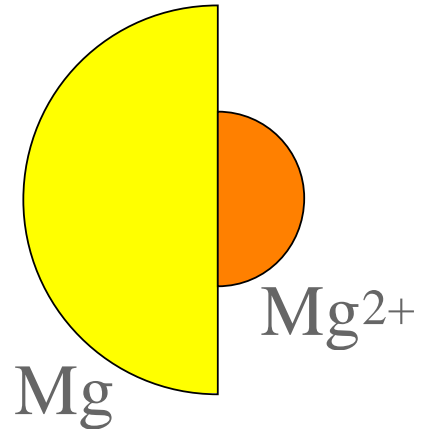
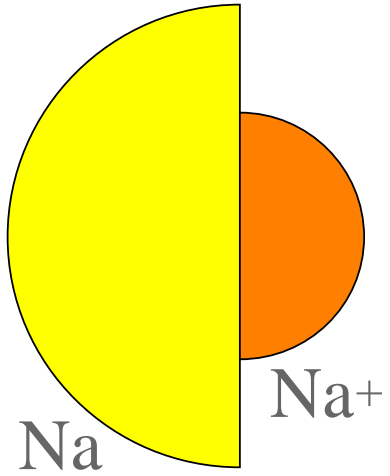
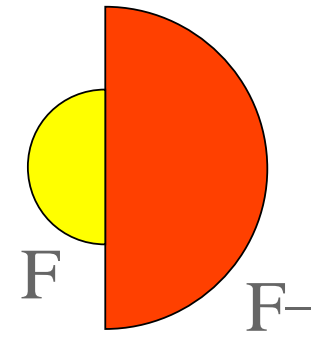
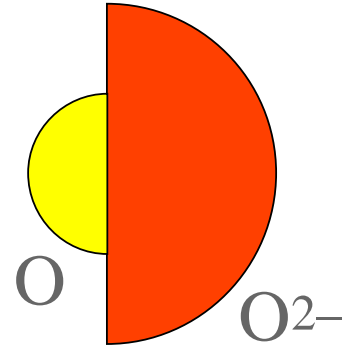
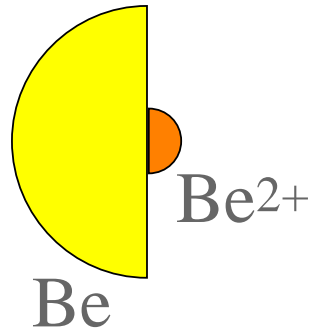
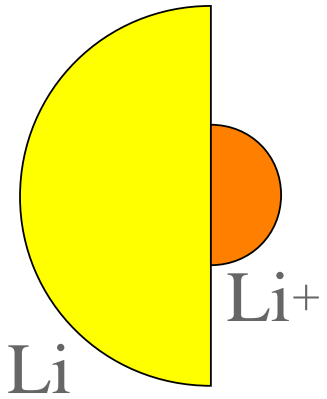
Término	Degeneración tno.	$J = L+S, \dots, L-S$	Símbolo nivel	Orientaciones de J	Degeneración nivel ($2J + 1$)
$1D$	5	$J = 2$	$1D_2$	$M_J = +2, +1, 0, -1, -2$	5 microestados
$3P$	9	$J = 2, 1, 0$	$3P_2$	$M_J = +2, +1, 0, -1, -2$	5 microestados
			$3P_1$	$M_J = +1, 0, -1$	3 microestados
			$3P_0$	$M_J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

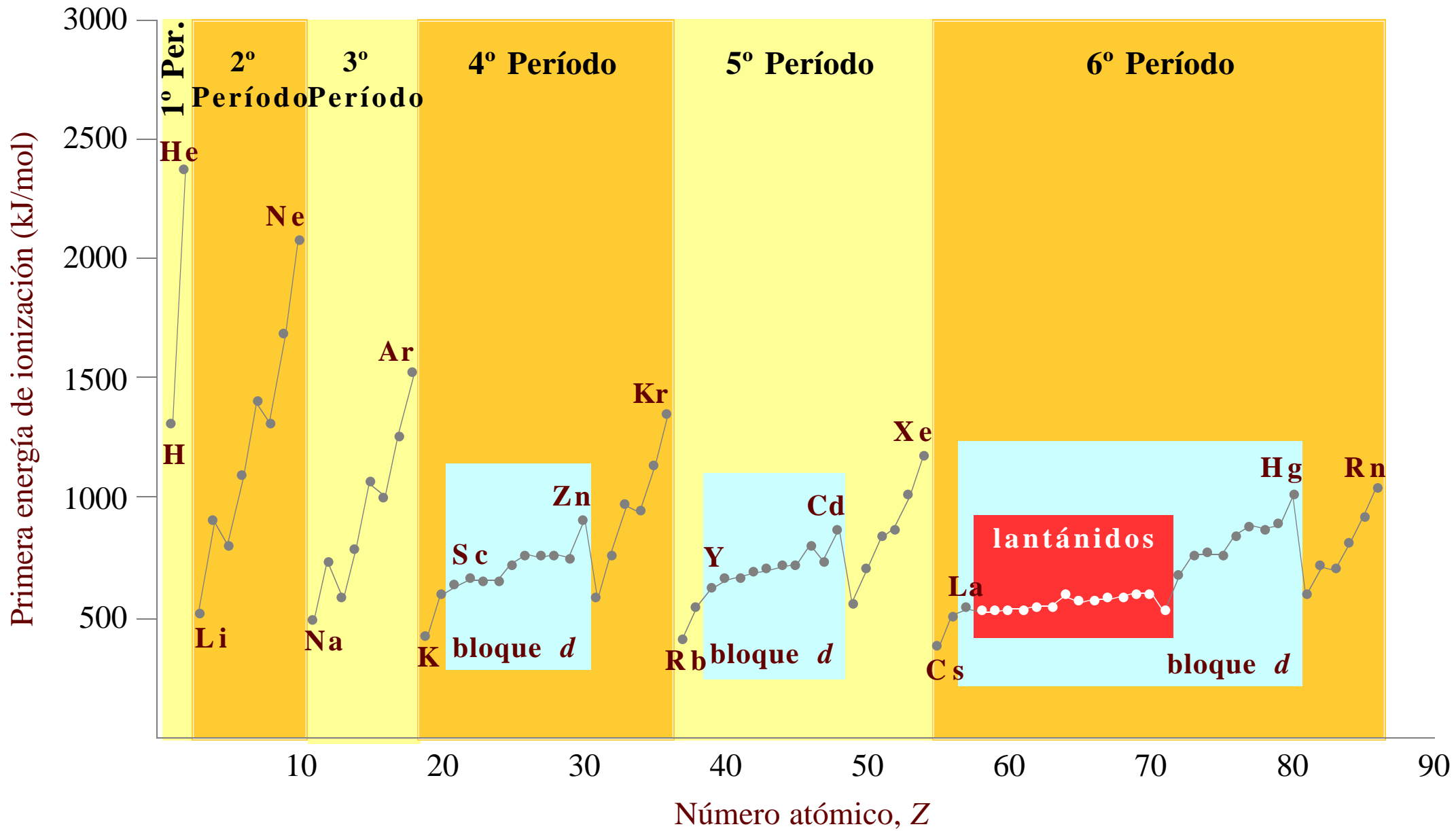




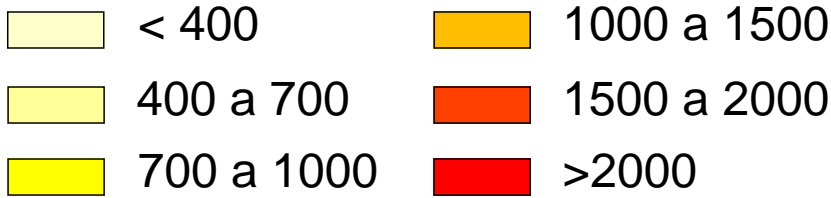


1Å





1												18																							
H 1310												He 2370																							
2												13 14 15 16 17																							
Li 519		Be 900												B 799		C 1090		N 1400		O 1310		F 1680		Ne 2080											
3		4		5		6		7		8		9		10		11		12		Al 577		Si 786		P 1060		S 1000		Cl 1260		Ar 1520					
Na 494		Mg 736		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	
K 418		Ca 590		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	
Rb 402		Sr 548		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	
Cs 376		Ba 502		Ac 666																															
Fr		Ra 509																																	



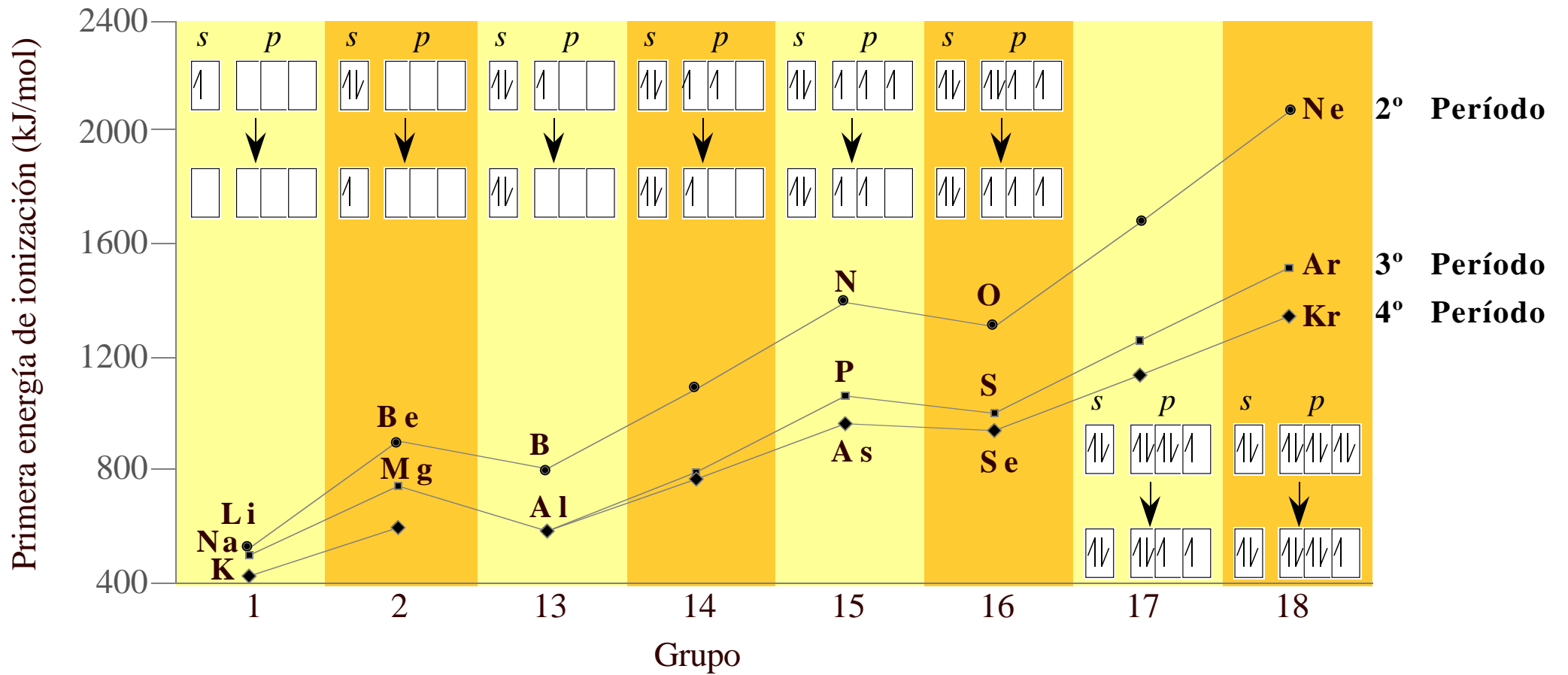


Tabla 1.14. Energías de ionización de los elementos del 2 al 5

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																
Na 53	Mg -230																
K 48	Ca -156																
Rb 47	Sr -167																
Cs 45	Ba -52																
Fr	Ra																

13	14	15	16	17	18
B 27	C 122	N 0	O 141	F 328	Ne -29
Al 42	Si 134	P 72	S 200	Cl 349	Ar -34
Ga 29	Ge 119	As 78	Se 195	Br 325	Kr -39
In 29	Sn 107	Sb 103	Te 190	I 295	Xe -40
Tl 19	Pb 35	Bi 91	Po 183	At 270	Rn -41

