

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

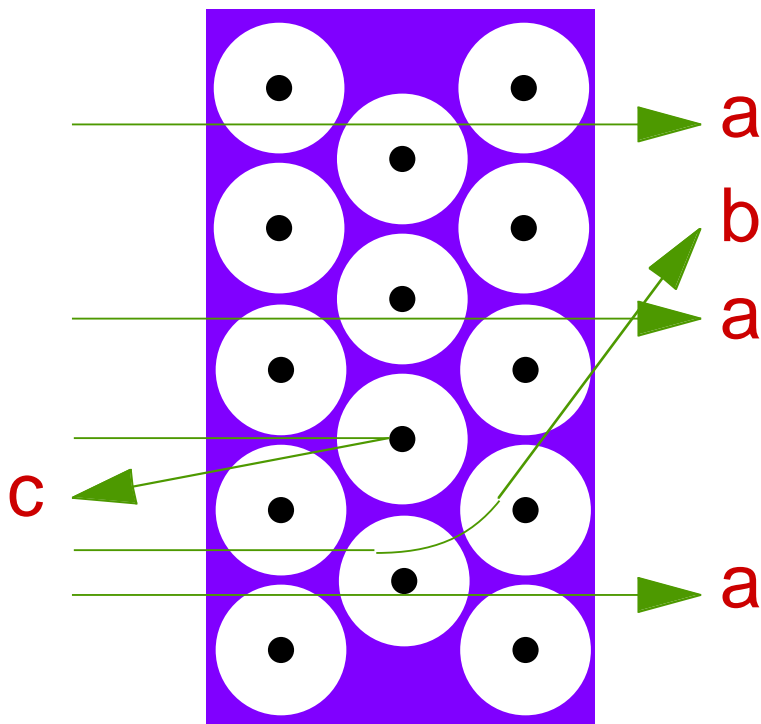
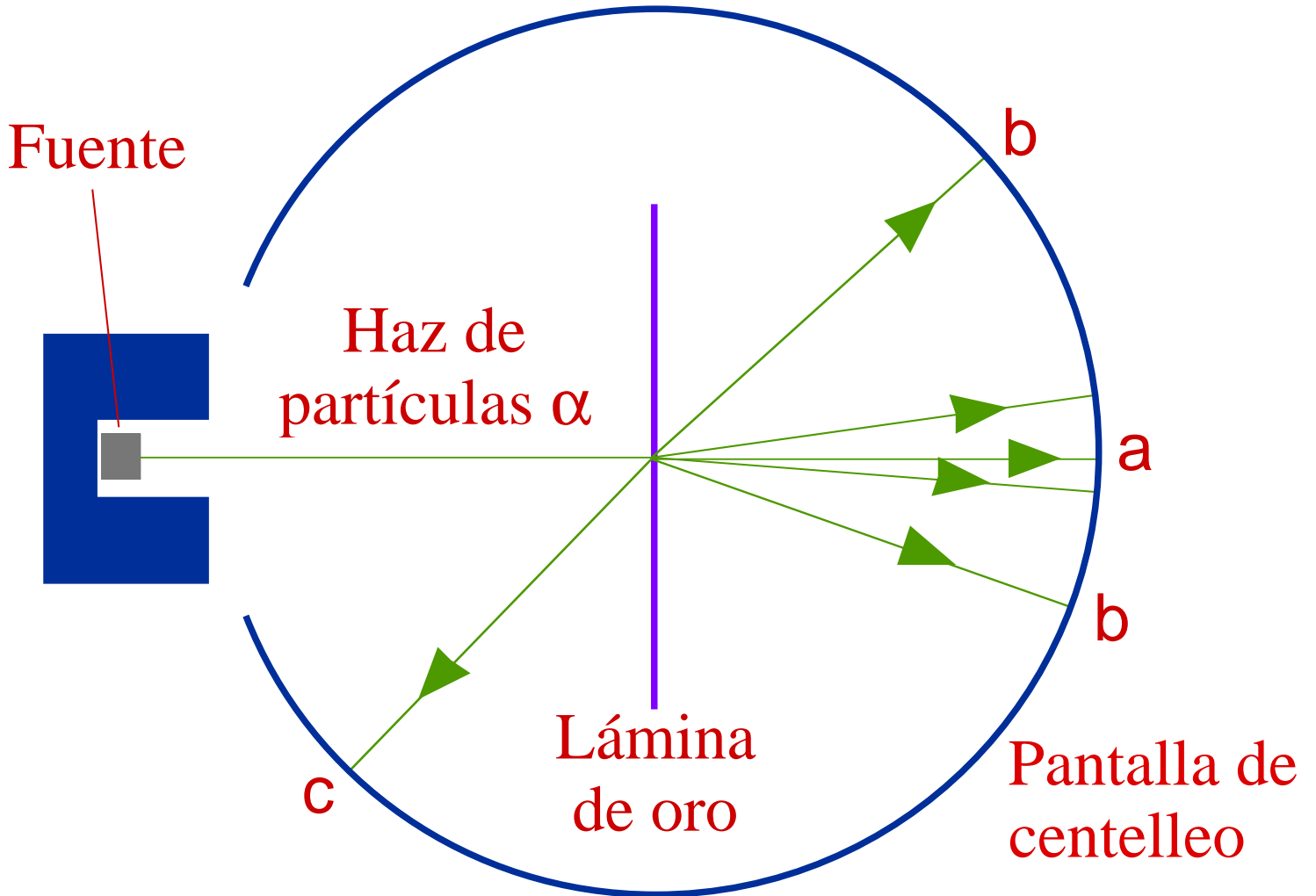
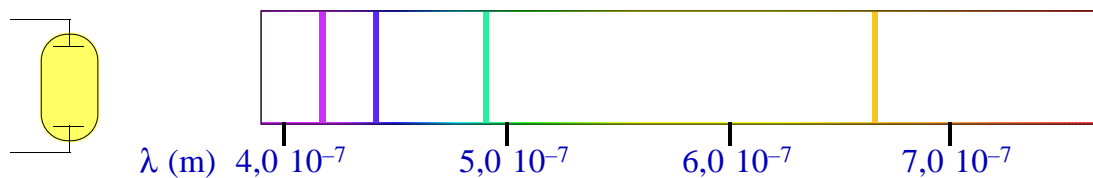
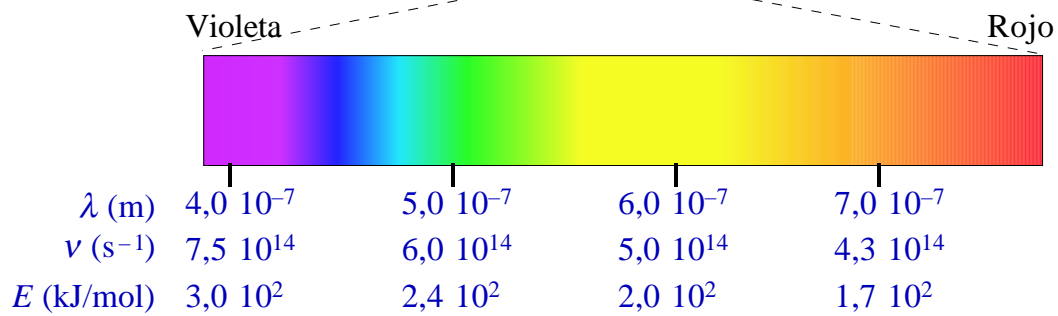
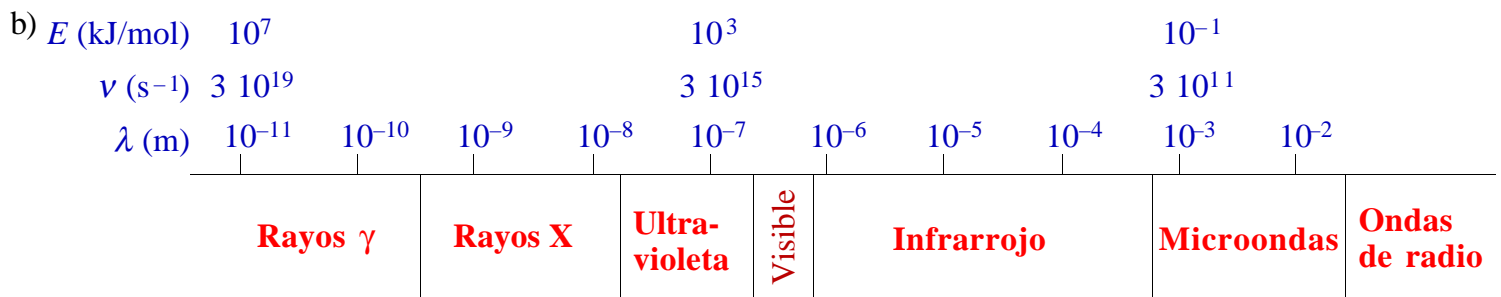
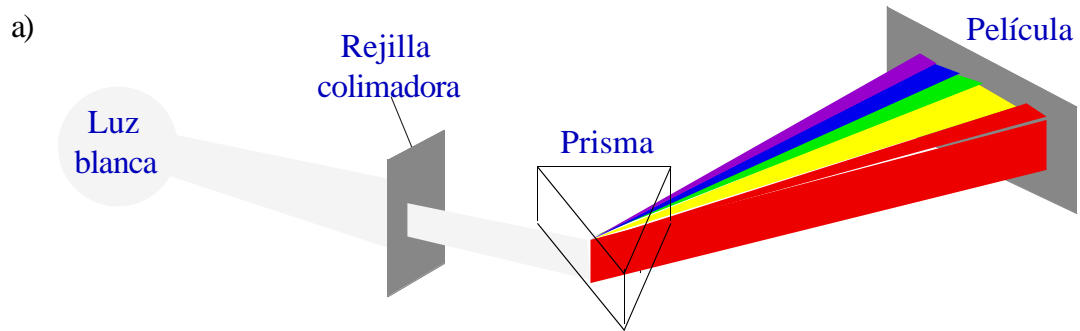
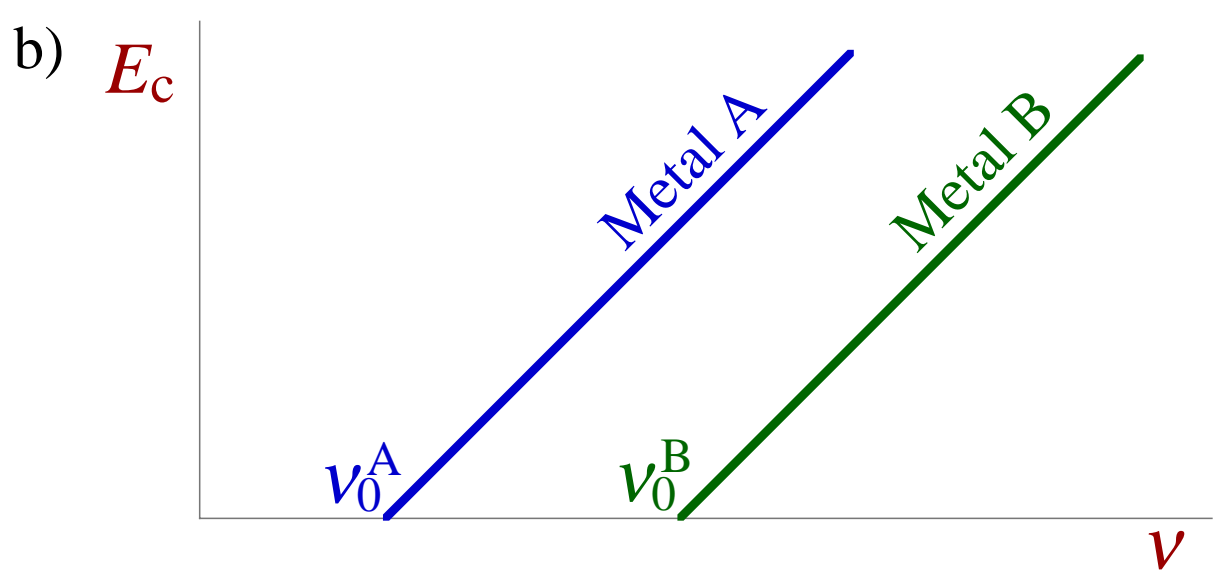
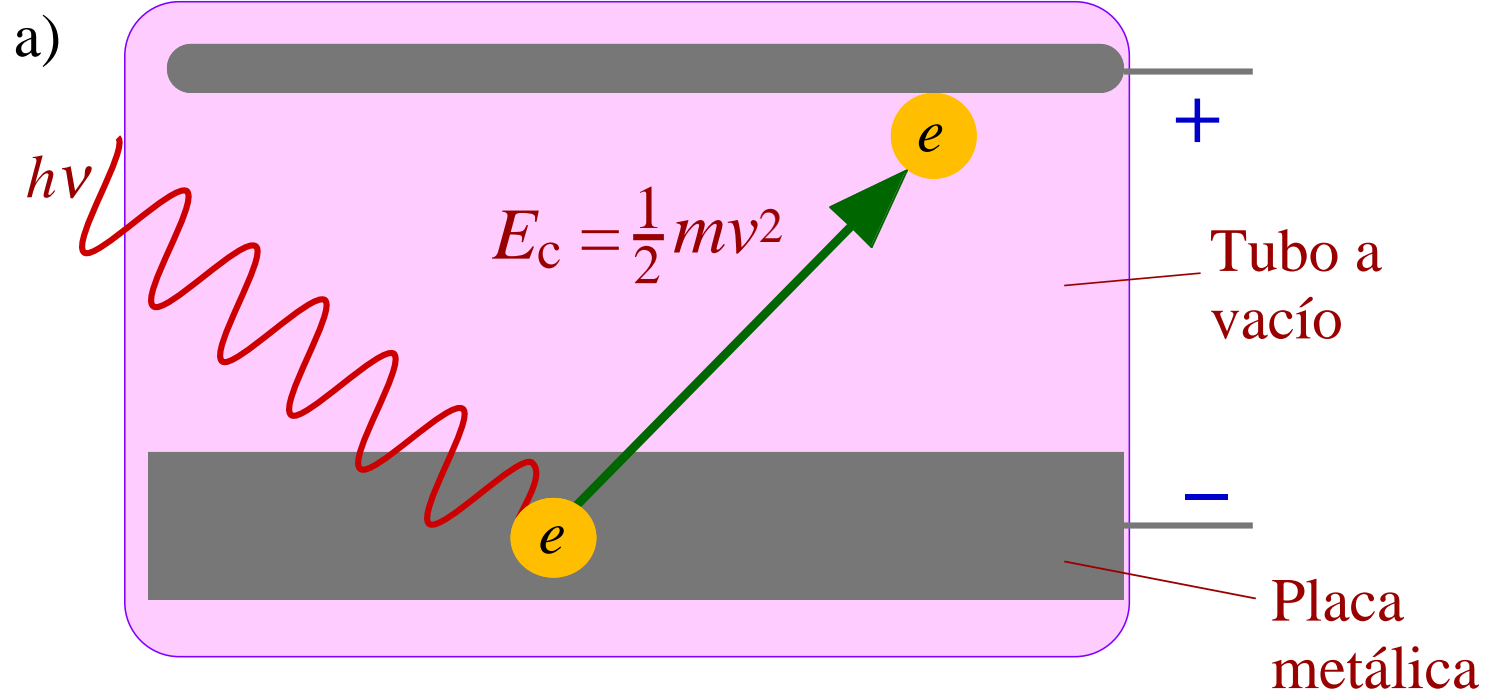
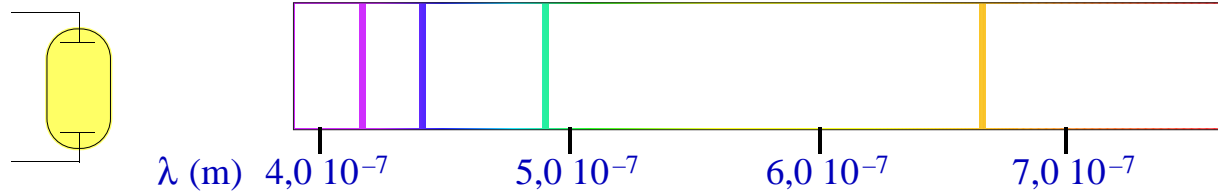


Tabla 1.2. Algunos elementos con varios isótopos

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



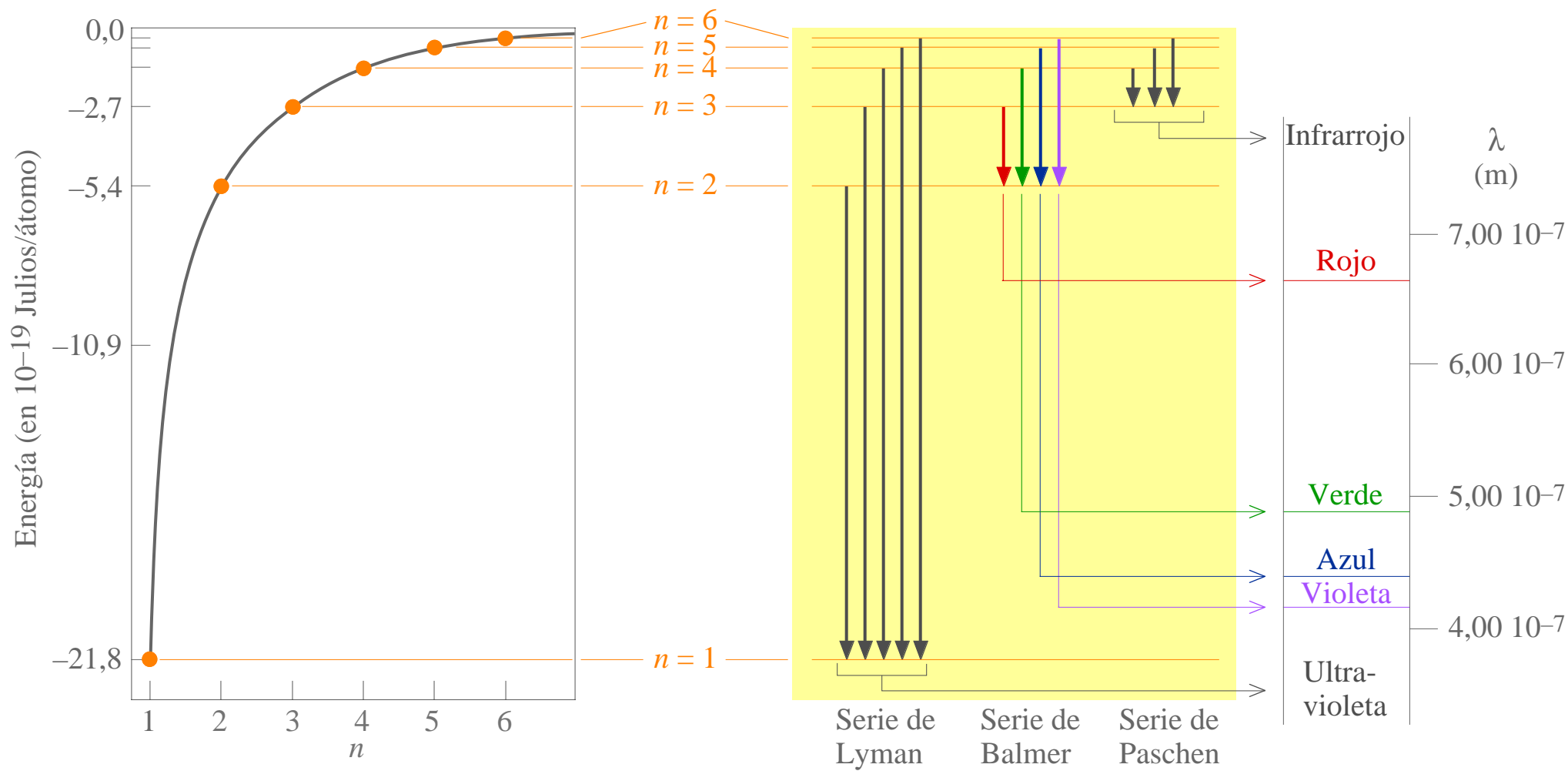




$$\nu = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

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



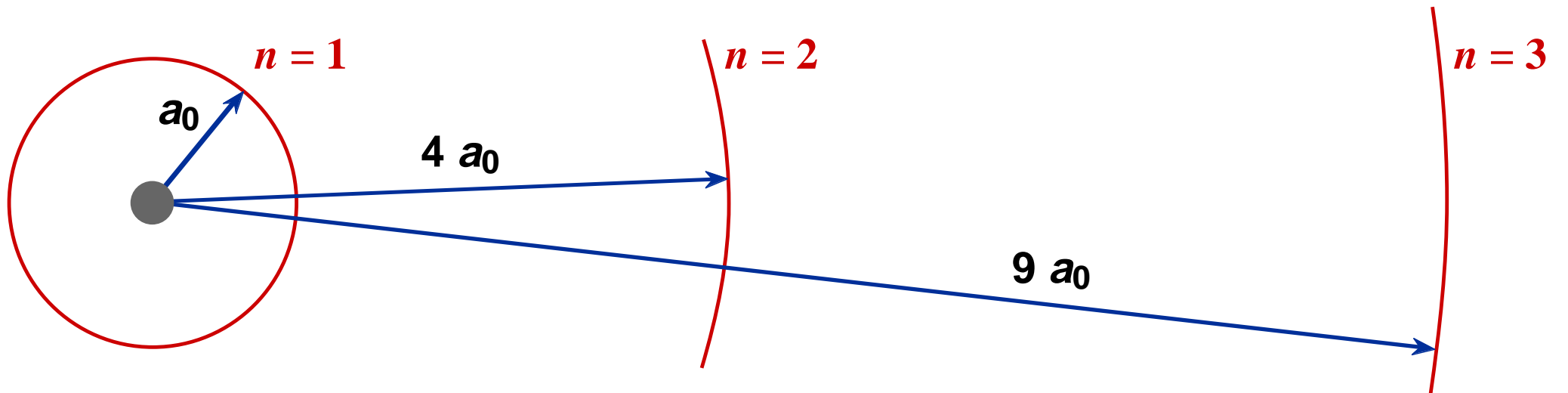


Tabla 1.3. Números cuánticos del átomo de hidrógeno

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

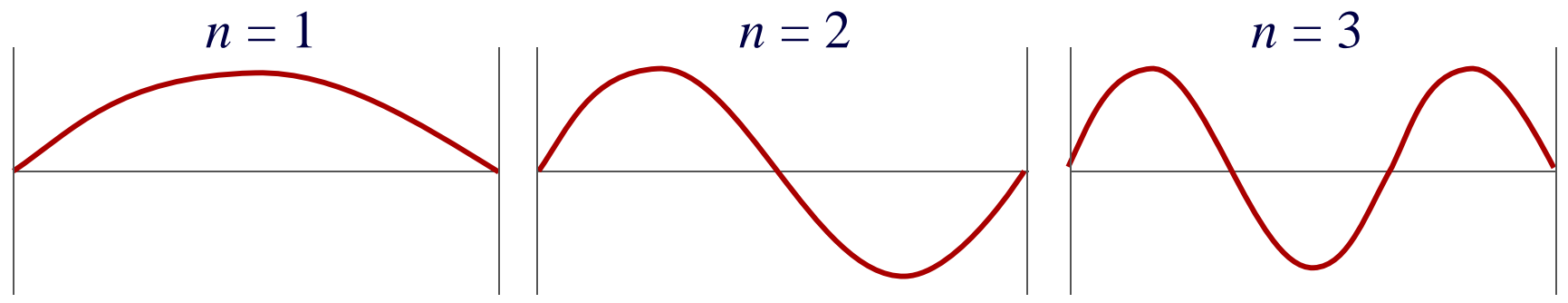
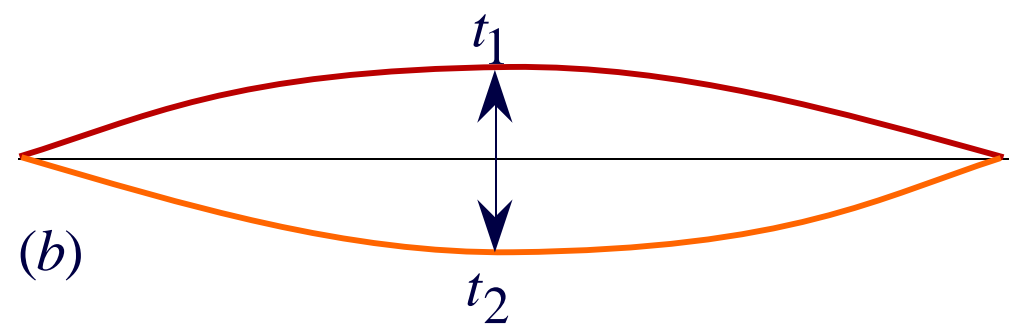
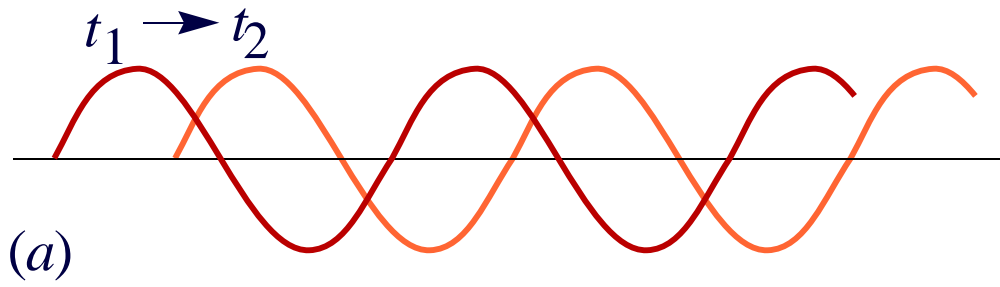
*También llamado momento angular orbital; ***órbita* en el lenguaje de Bohr, *orbital* en el de la mecánica cuántica.

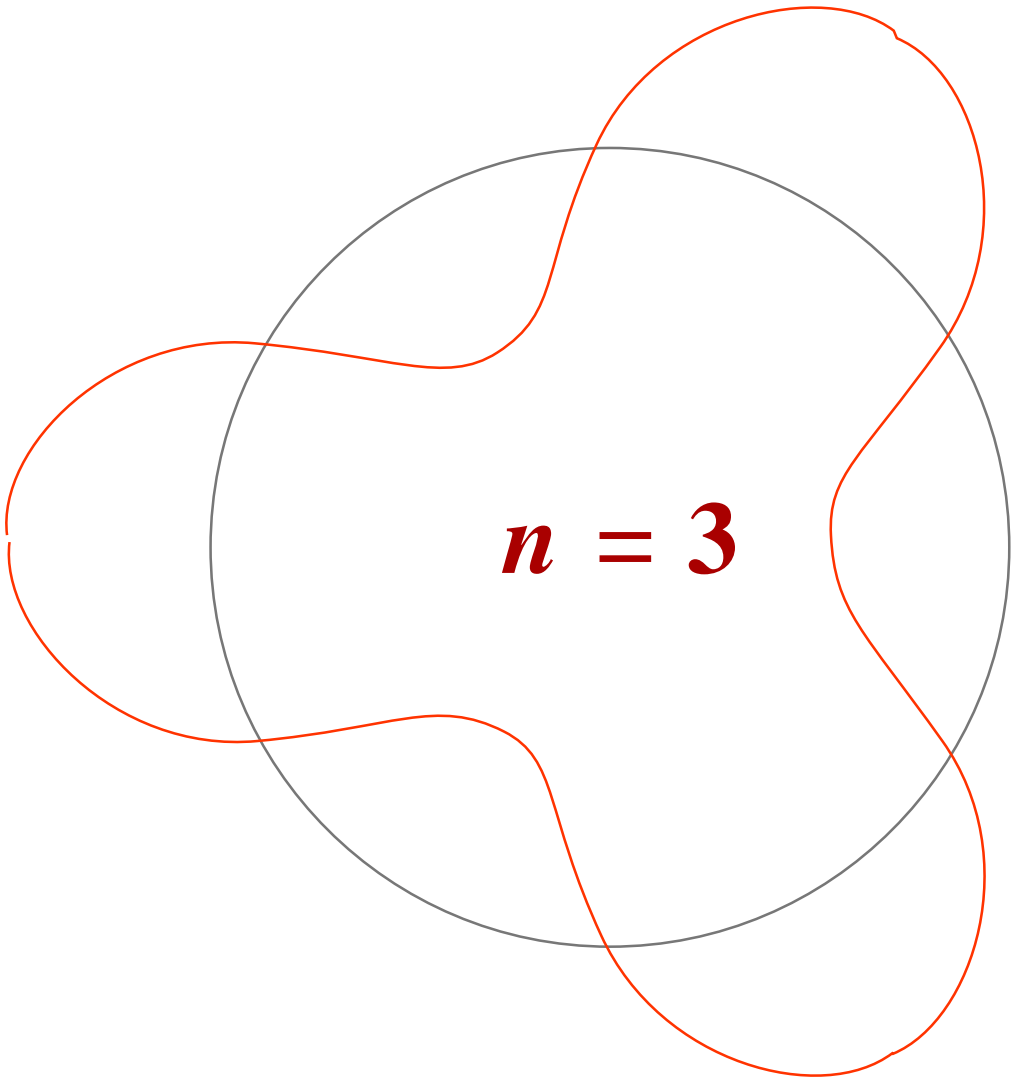
Tabla 1.4. Longitudes de onda de partículas

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	$3,3 \cdot 10^{-24}$

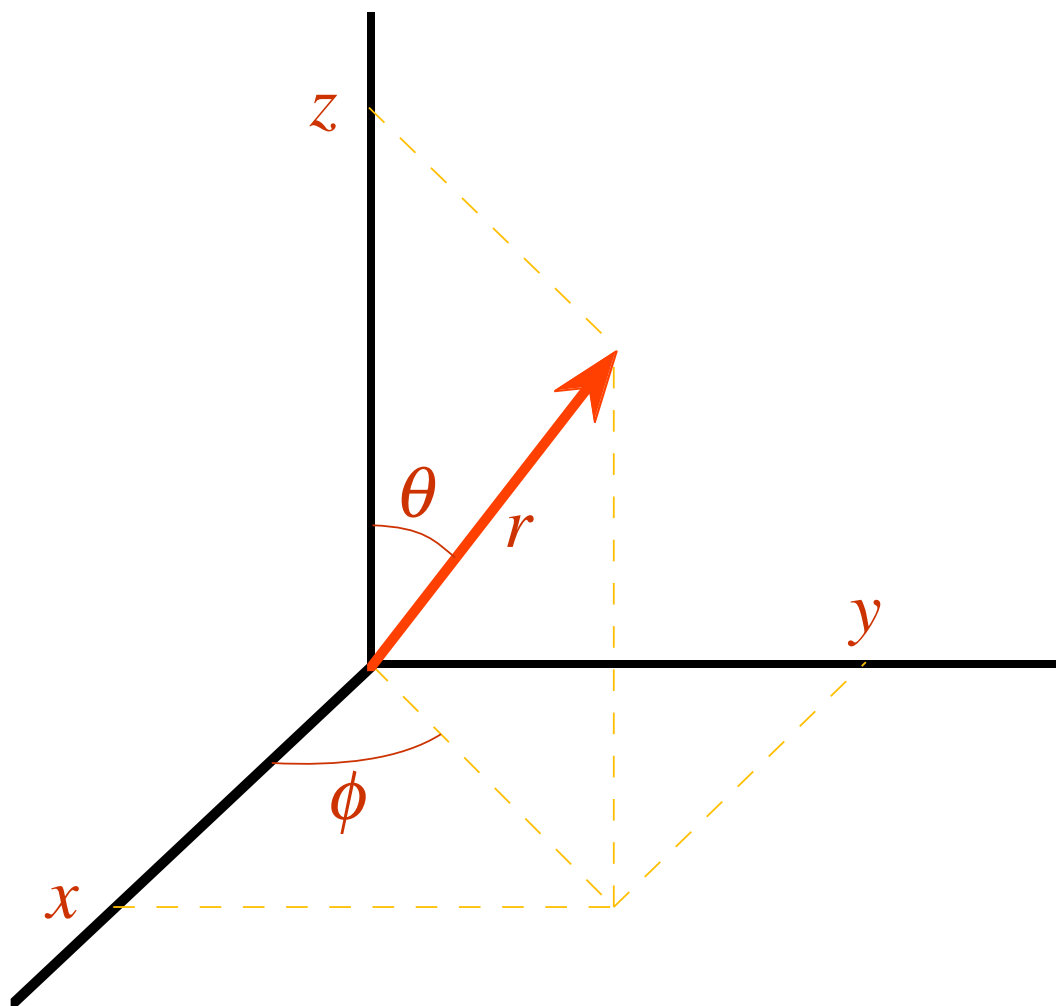
Ejemplo. Imprecisión mínima en la posición de partículas cuya imprecisión en la velocidad es del 1%

<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

$$z = r \cos \theta$$

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

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

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

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

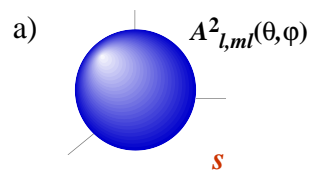
$$\phi = \arctg(y/x)$$

Tabla 1.5. 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

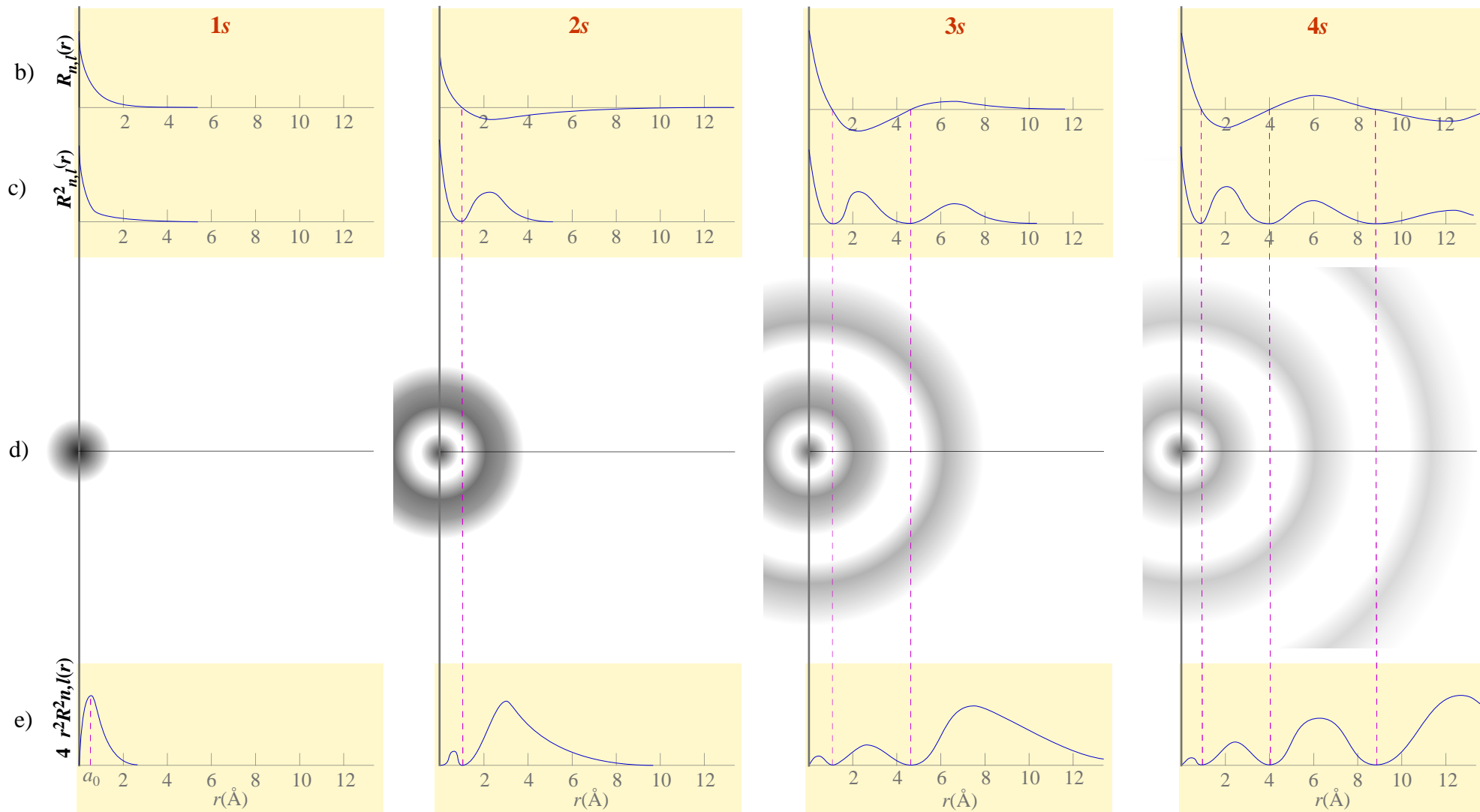
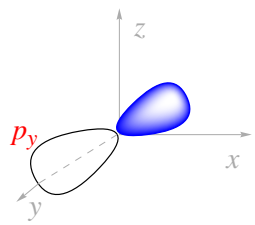
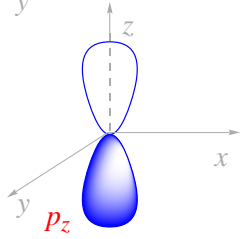
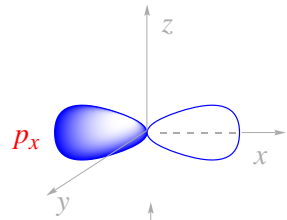


Tabla 1.6. Funciones angulares A_{l,m_l} normalizadas para átomos o iones monoelectrónicos

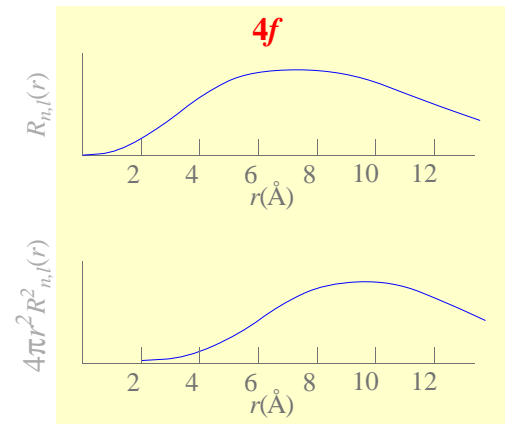
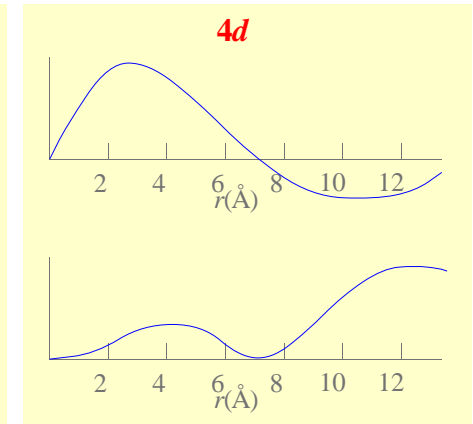
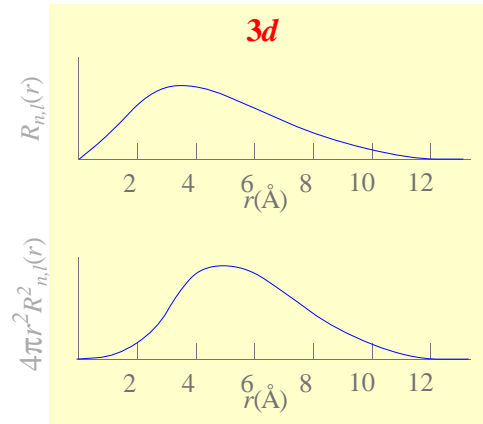
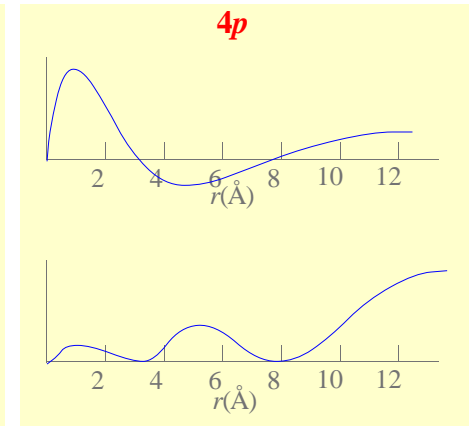
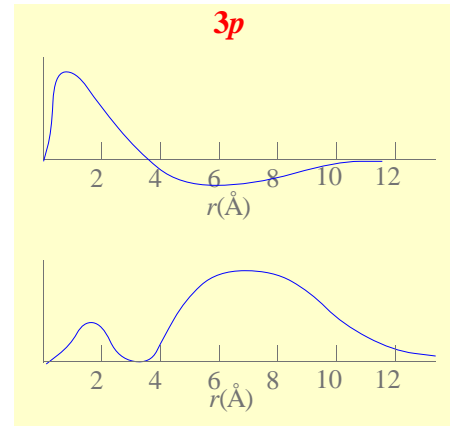
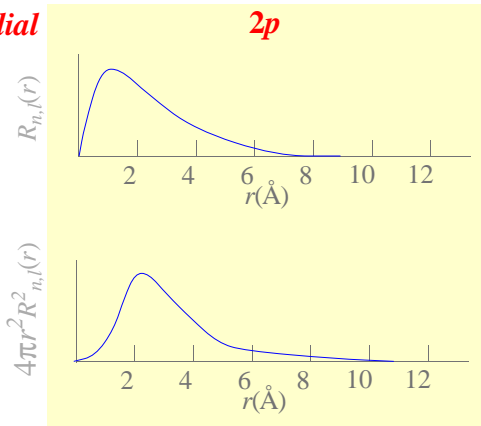
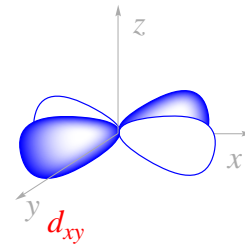
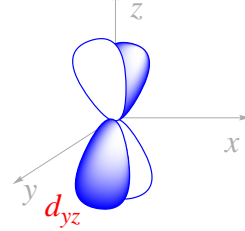
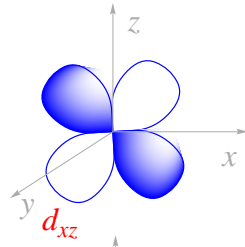
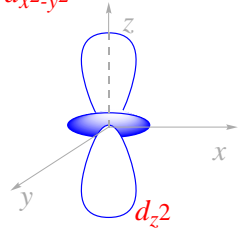
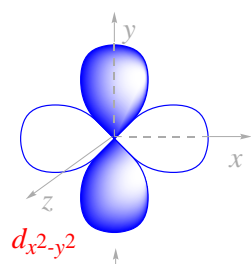
Orbital	$A_{l,m_l}(\theta, \phi)^*$	$A_{l,m_l}(x, y, z)^{**}$
s	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
p_z	$\frac{\sqrt{3}}{2\sqrt{\pi}} \cos \theta$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (z/r)$
p_x	$\frac{\sqrt{3}}{2\sqrt{\pi}} \text{sen } \theta \cos \phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}} (x/r)$
p_y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

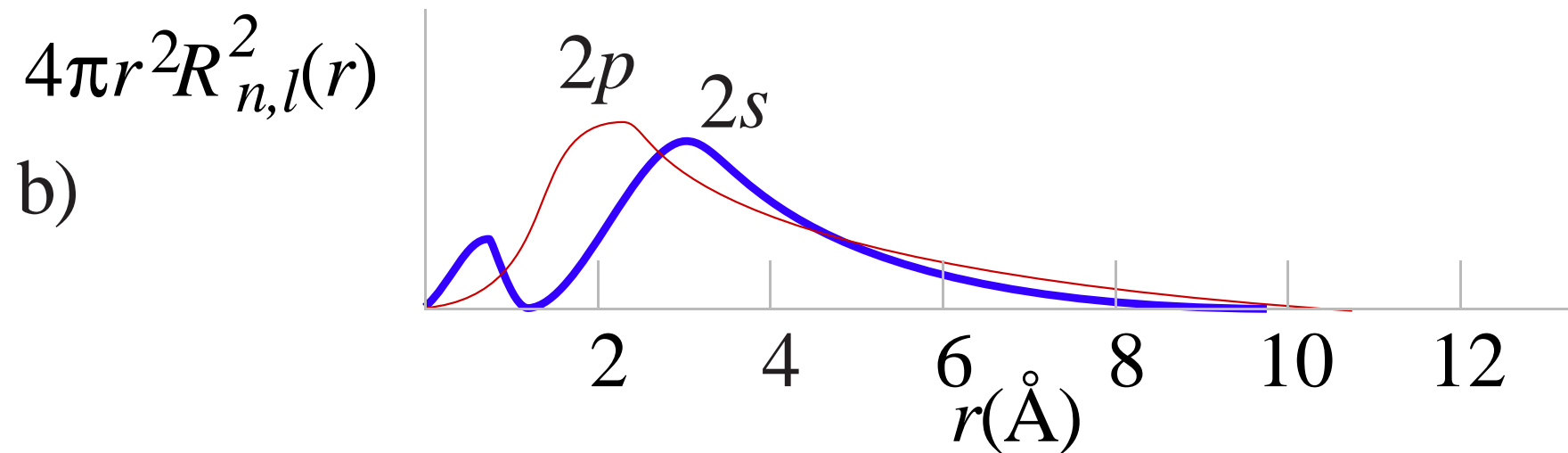
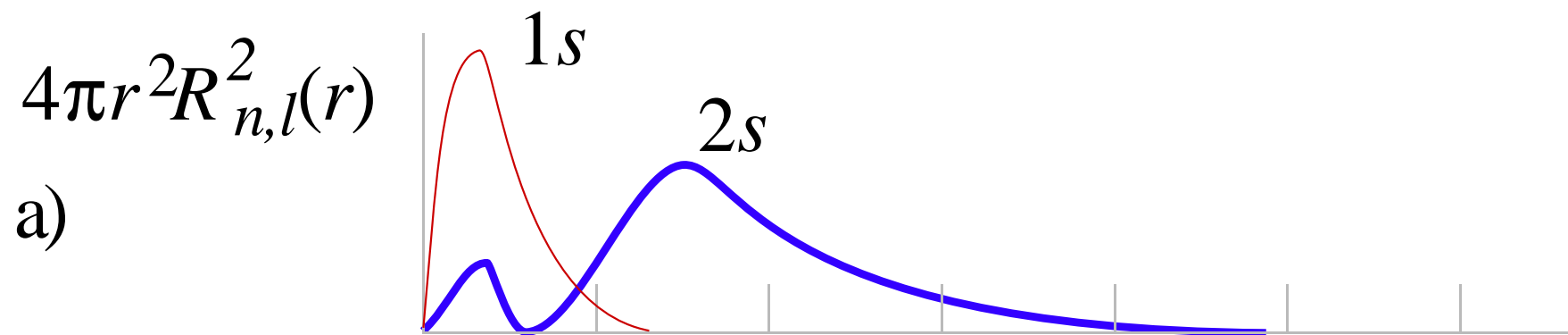
* Funciones en el sistema de coordenadas polares esféricas. ** Funciones en el sistema de coordenadas cartesiano.

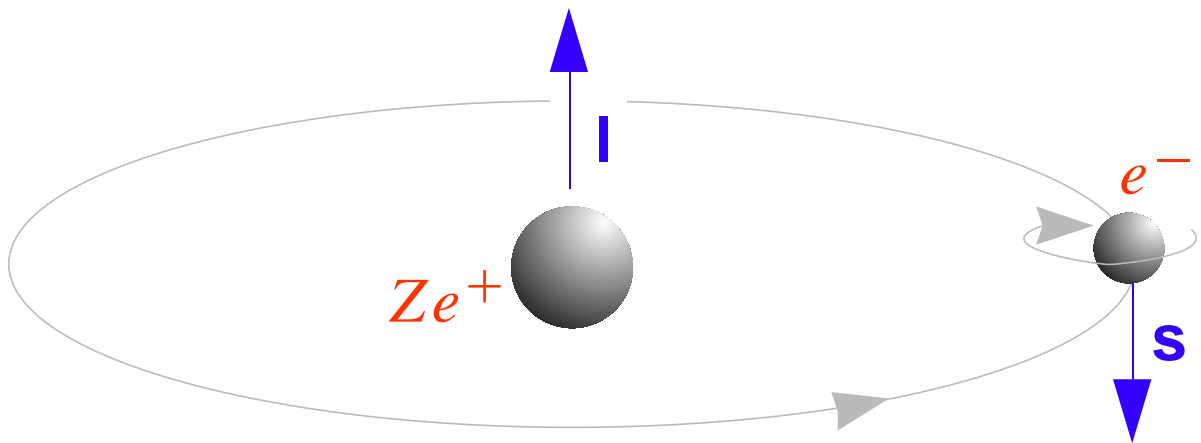
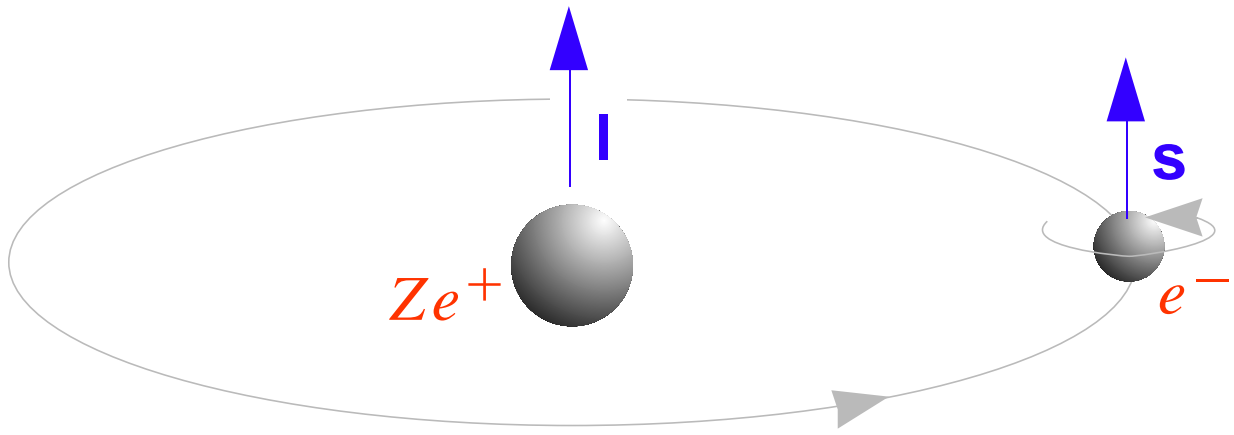
Parte Angular

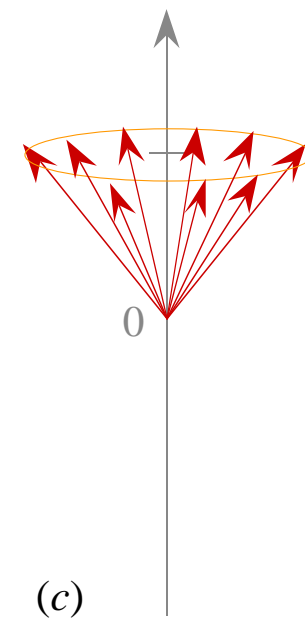
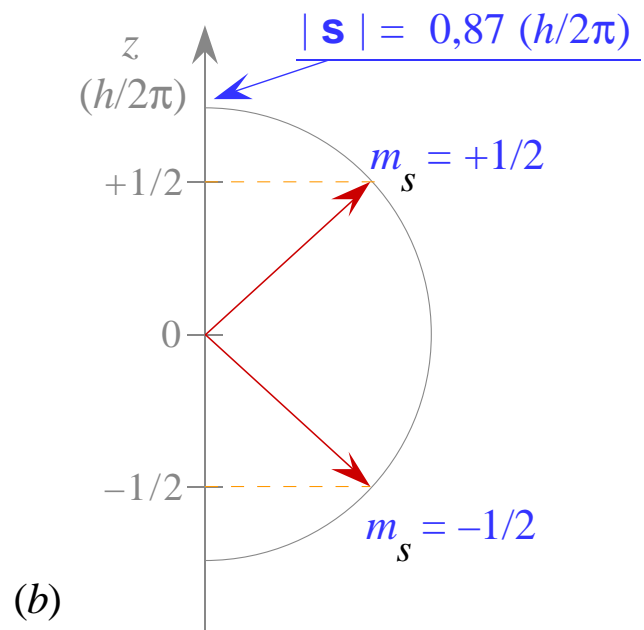
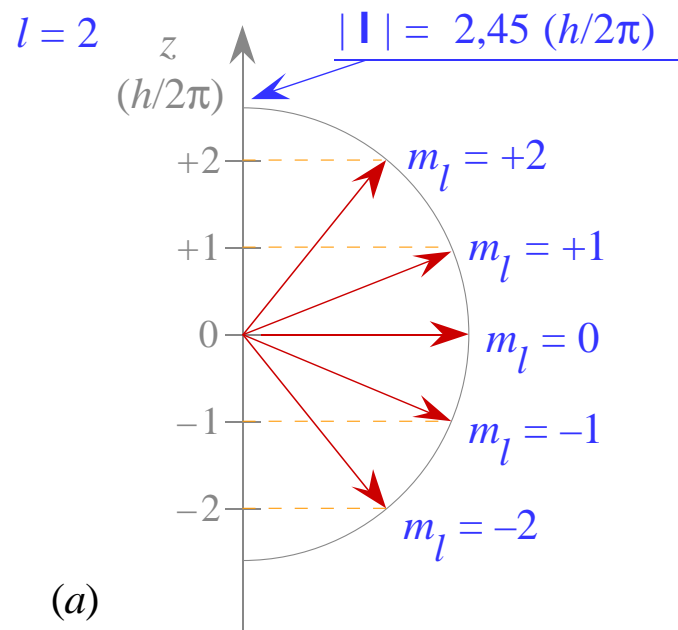


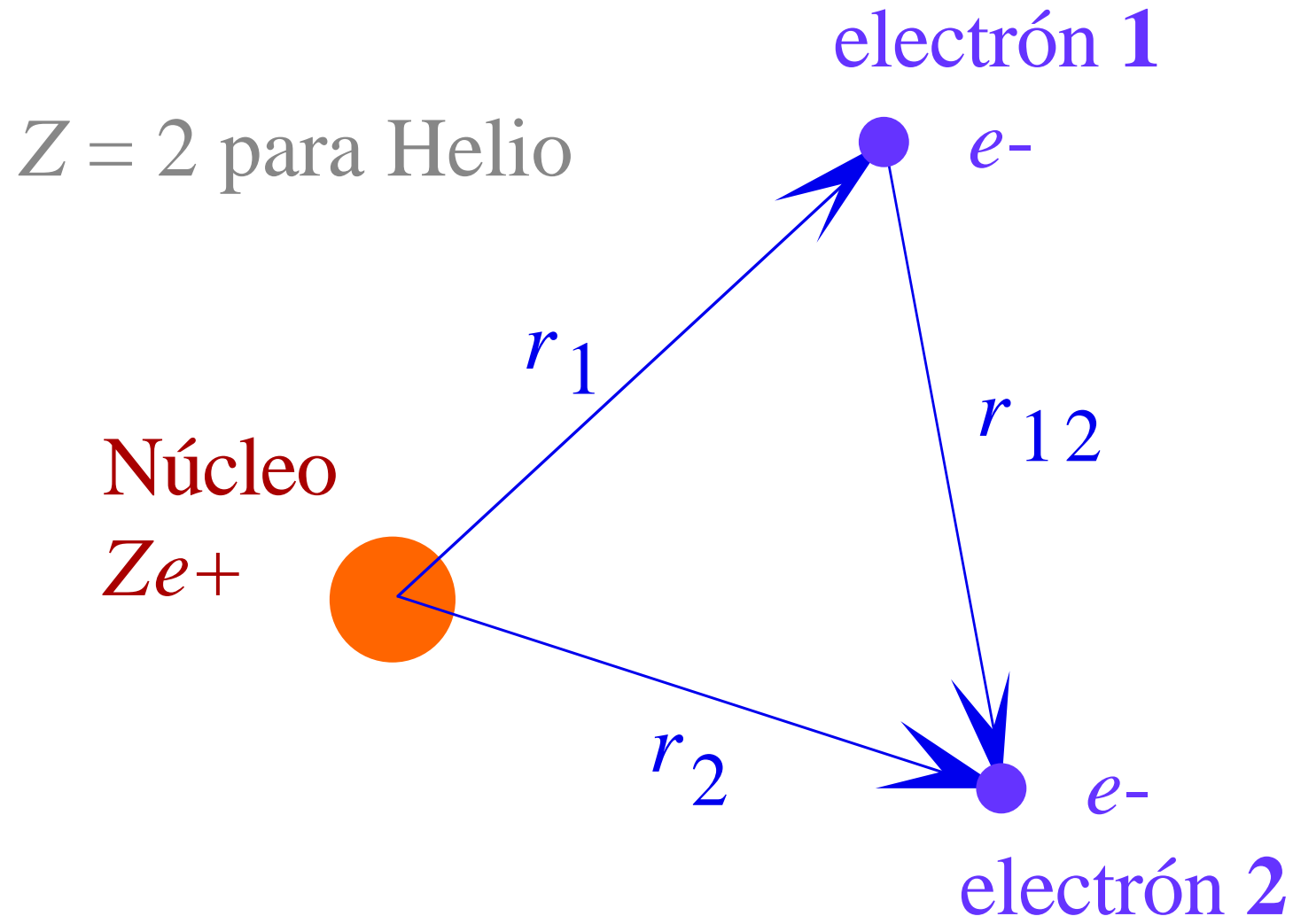
Parte Radial











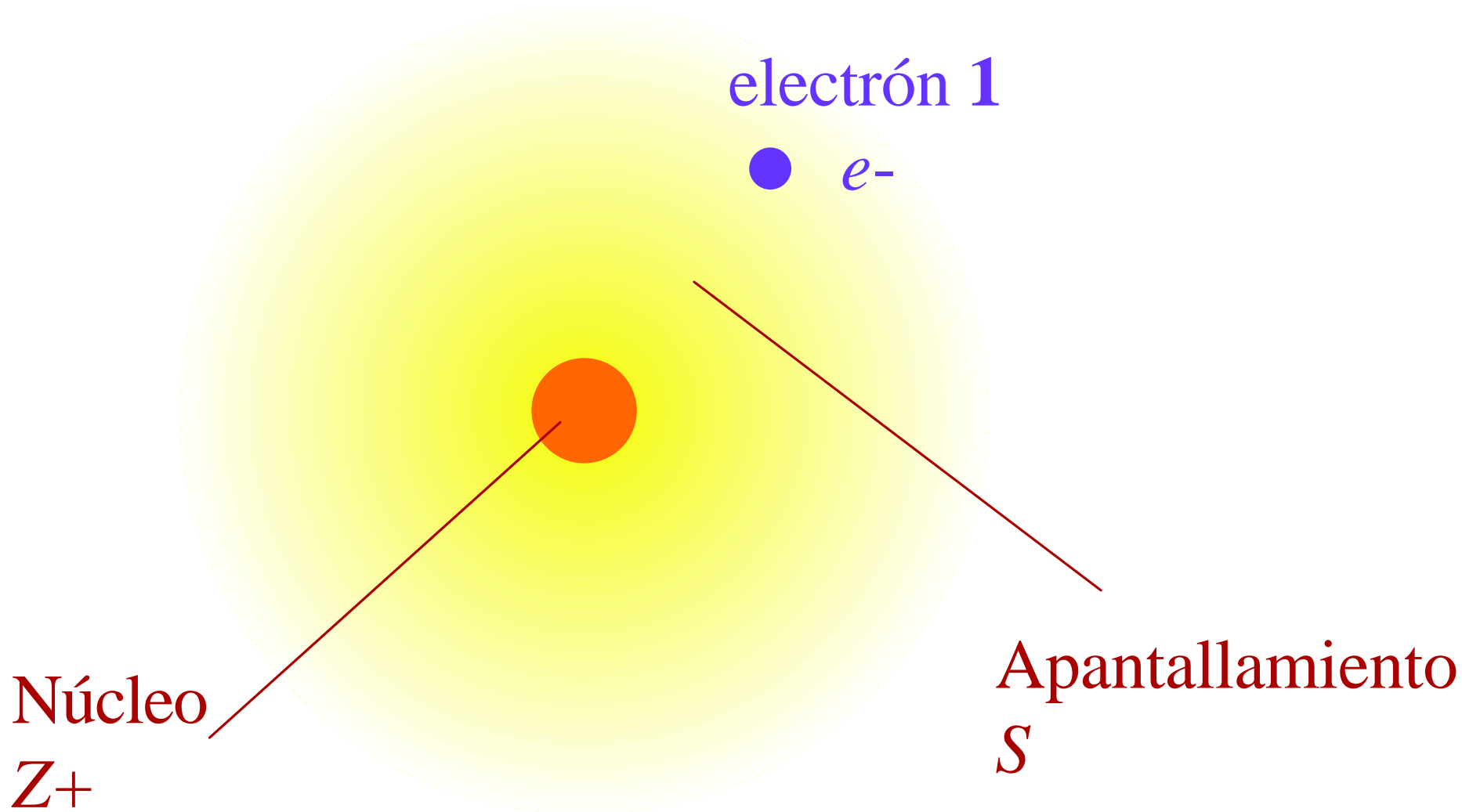
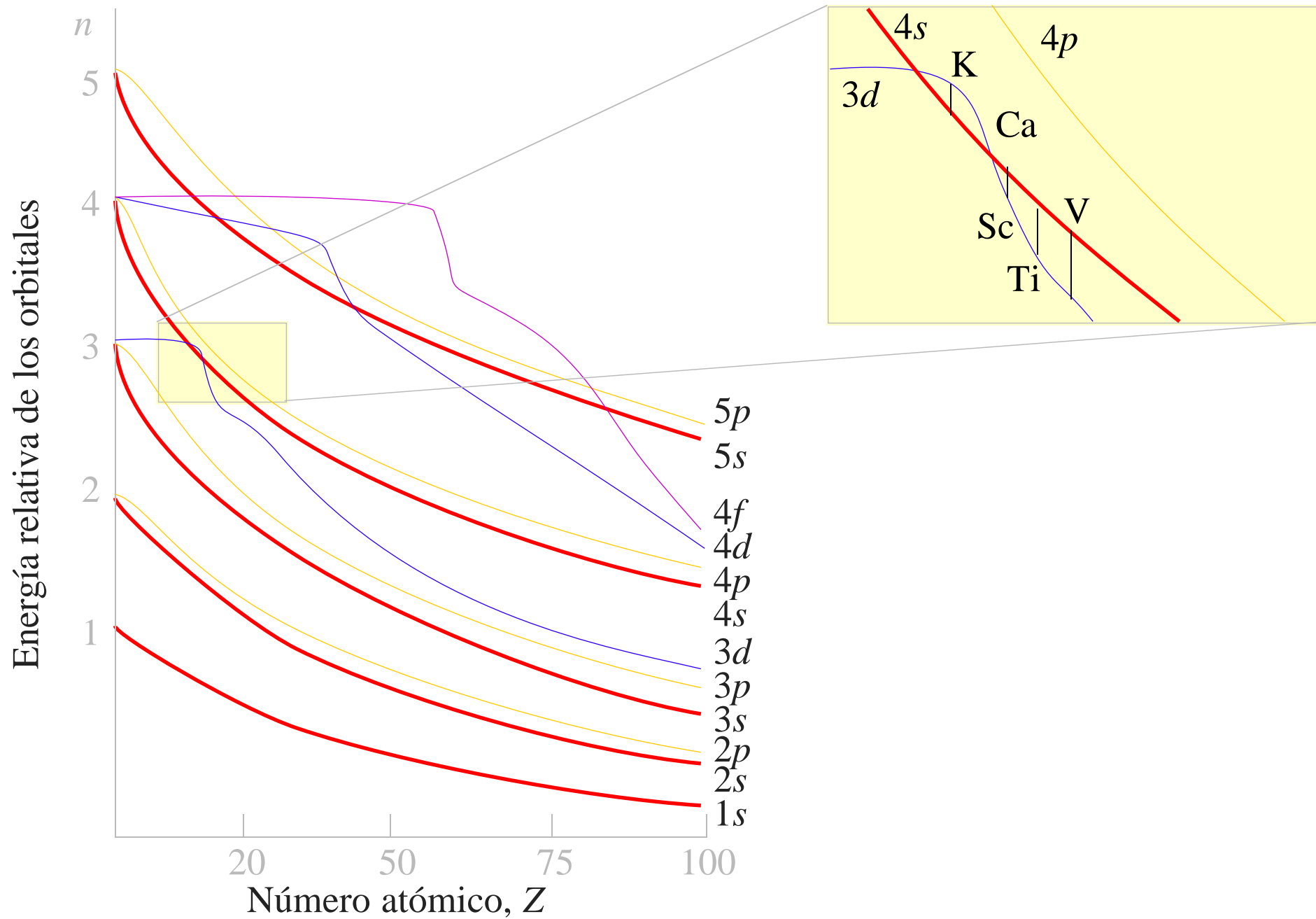


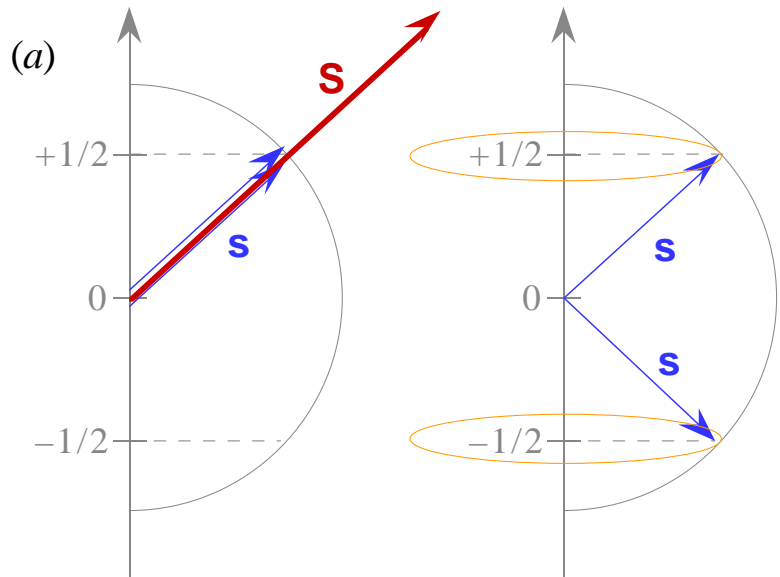
Tabla 1.7 (parcial). Cargas Nucleares Efectivas de los elementos del 1 al 36

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

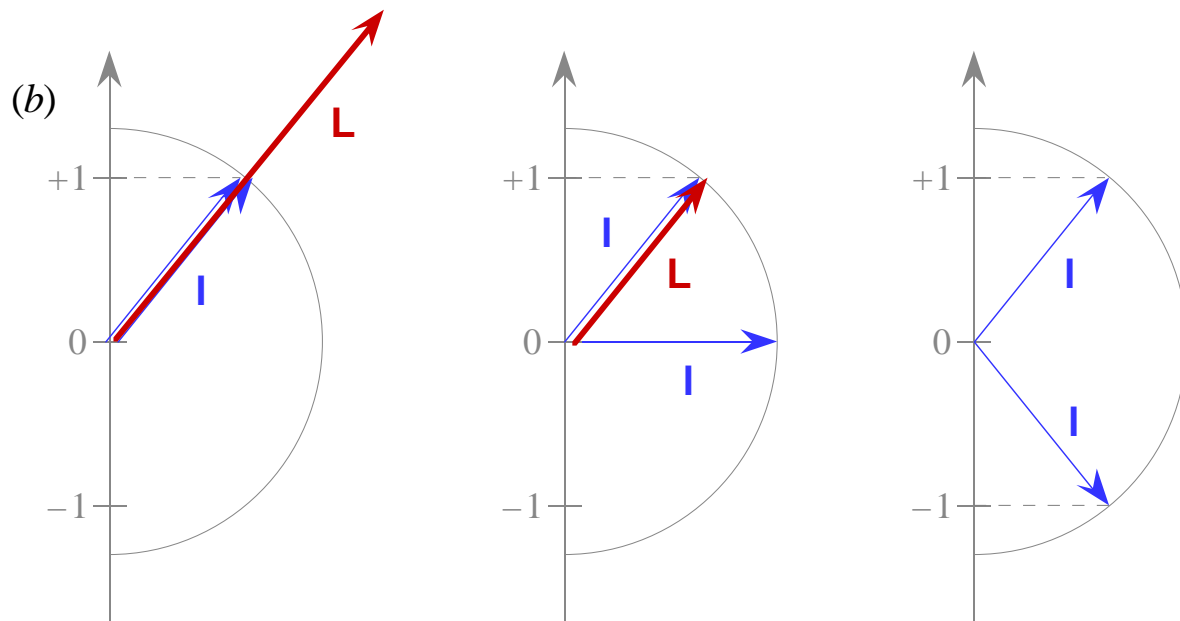
Tipo de función de onda		Energía (en eV)
1	Producto de orbitales del He ⁺ (aprox. orbital)	-74,83
2	Producto de orbitales con Z* fijada por el método SCF	-77,48
3	Producto de funciones más apropiado	-77,870917
4	Función no orbitalaria de Pekeris (combinación lineal de 1078 términos)	-79,00946912
	Valor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





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

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



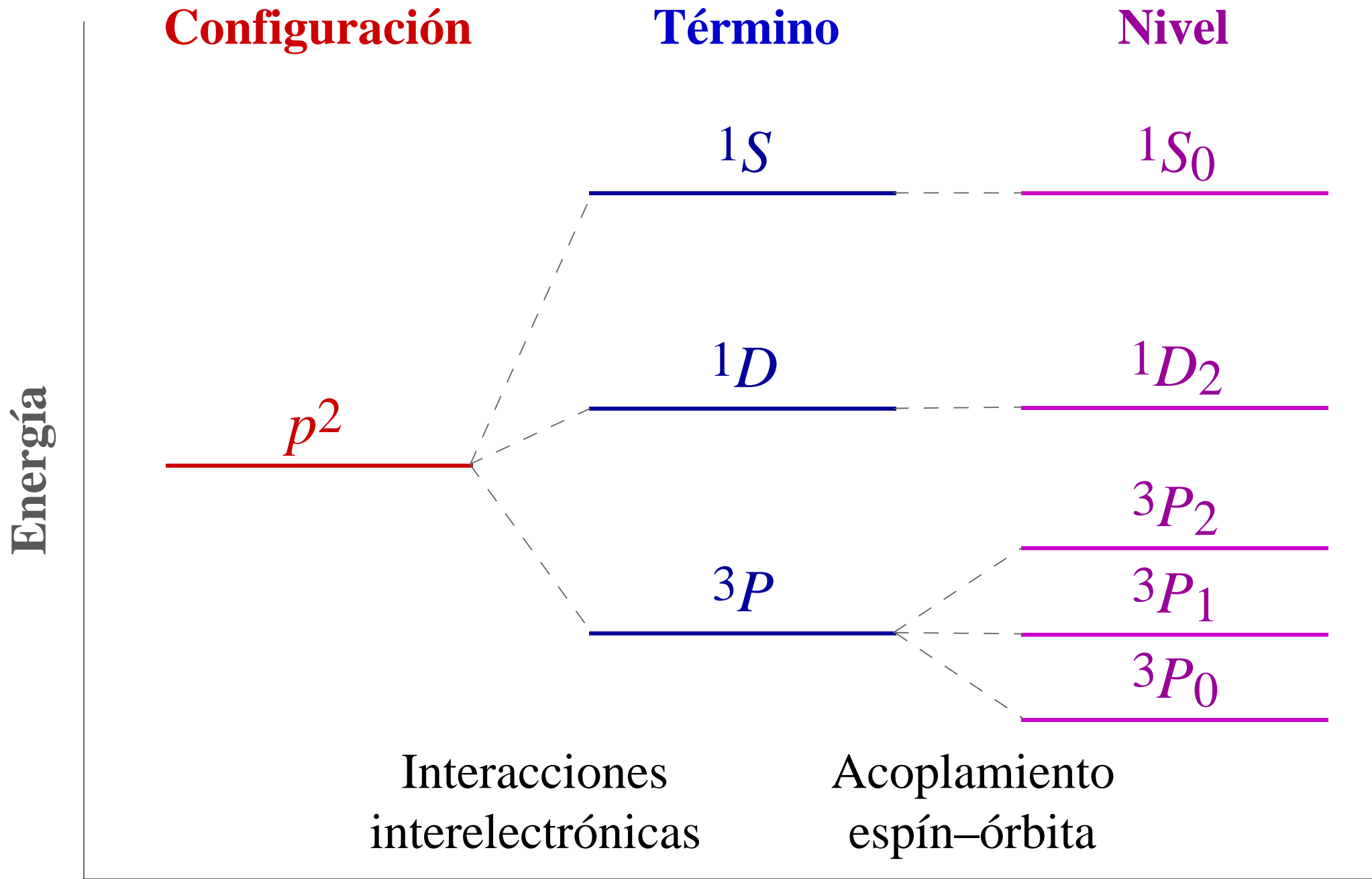
$l = 1$
 $L = 2$
 $M_L = +2, +1, 0, -1, -2$

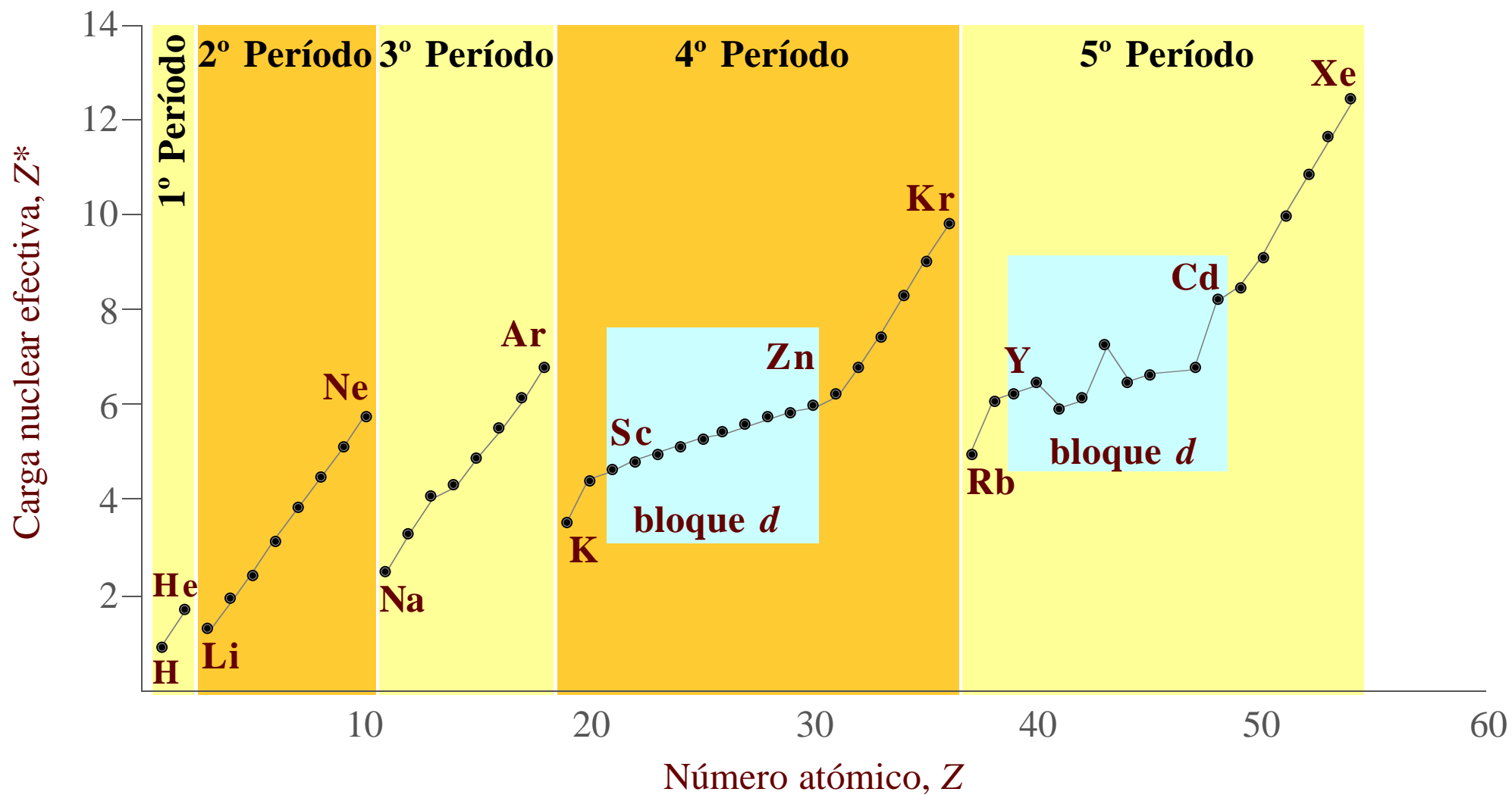
$l = 1$
 $L = 1$
 $M_L = +1, 0, -1$

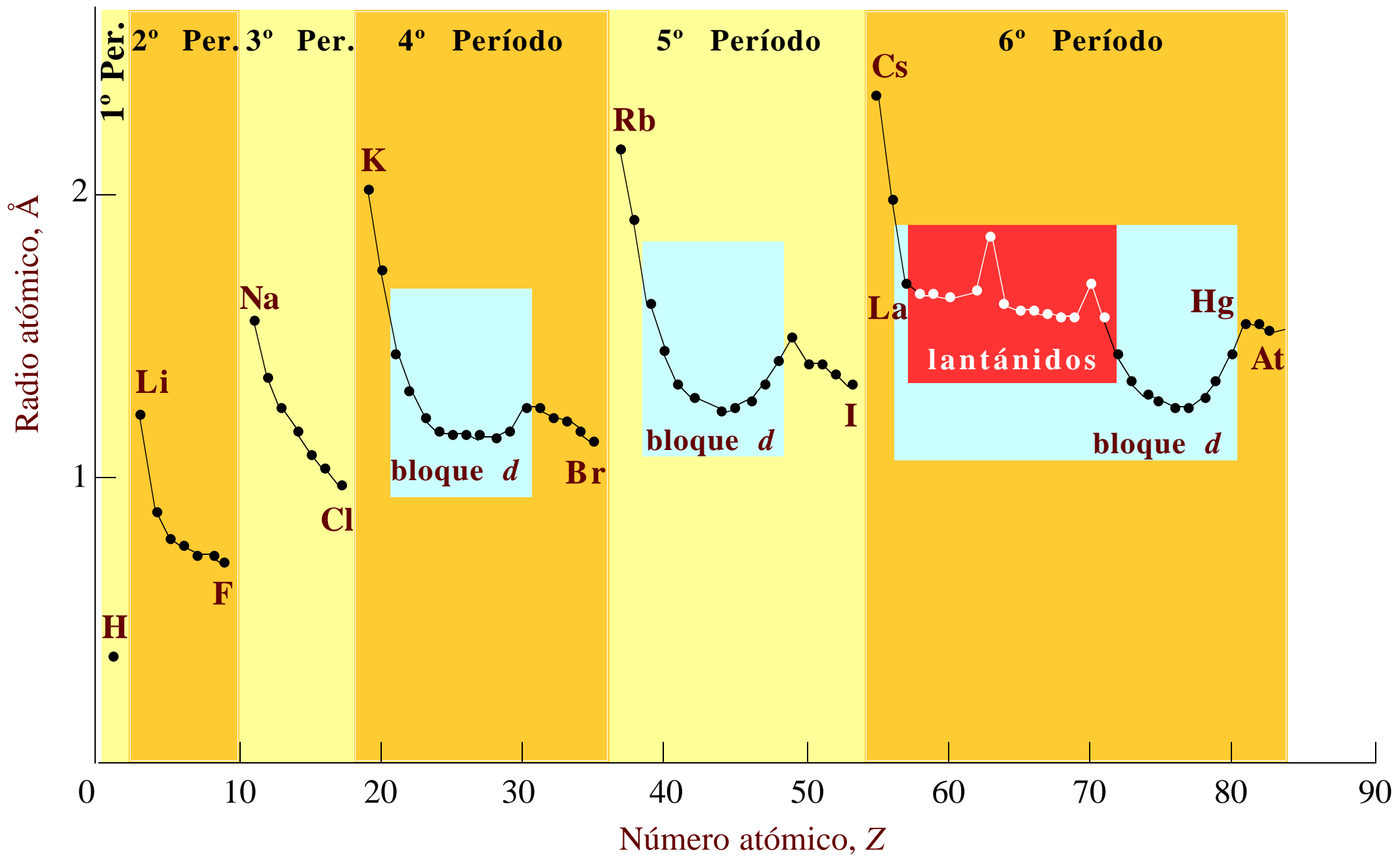
$l = 1$
 $L = 0$
 $M_L = 0$

Tabla 1.10. Términos Russell–Saunders para algunas configuraciones

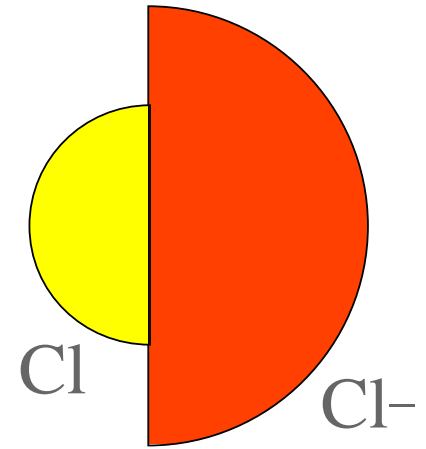
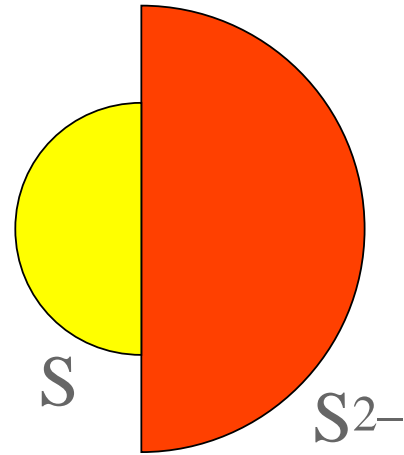
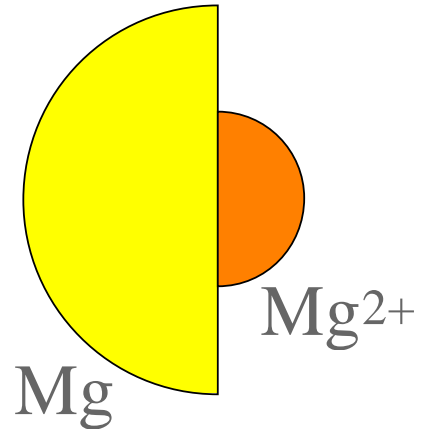
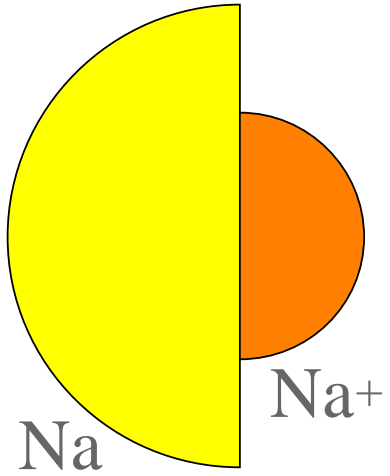
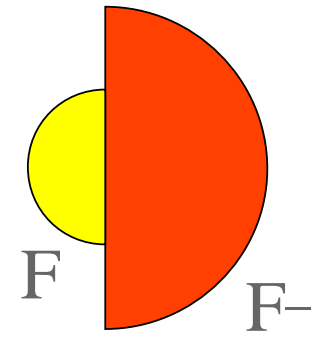
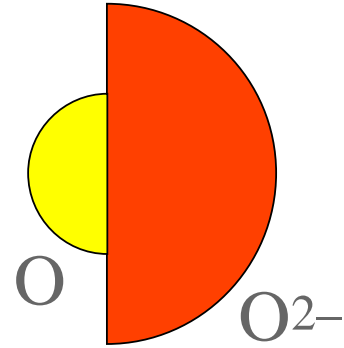
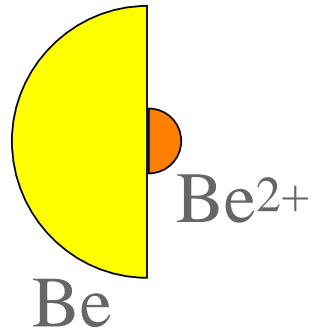
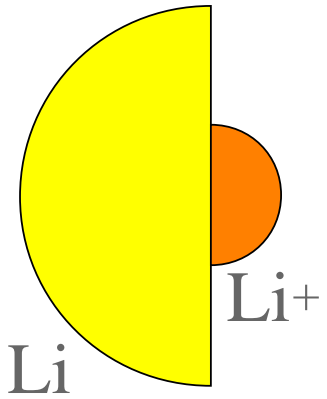
Configuración	Términos	Término fundamental
s^1	2S	2S
s^2	1S	1S
p^1 y p^5	2P	2P
p^2 y p^4	$^1S, ^1D, ^3P$	3P
p^3	$^2P, ^2D, ^4S$	4S
p^6	1S	1S
d^1 y d^9	2D	2D
d^2 y d^8	$^1S, ^1D, ^1G, ^3P, ^3F$	3F
d^3 y d^7	$^2P, ^2D(2), ^2F, ^2G, ^2H, ^4P, ^4F$	4F
d^4 y d^6	$^1S(2), ^1D(2), ^1F, ^1G(2), ^1I, ^3P(2),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

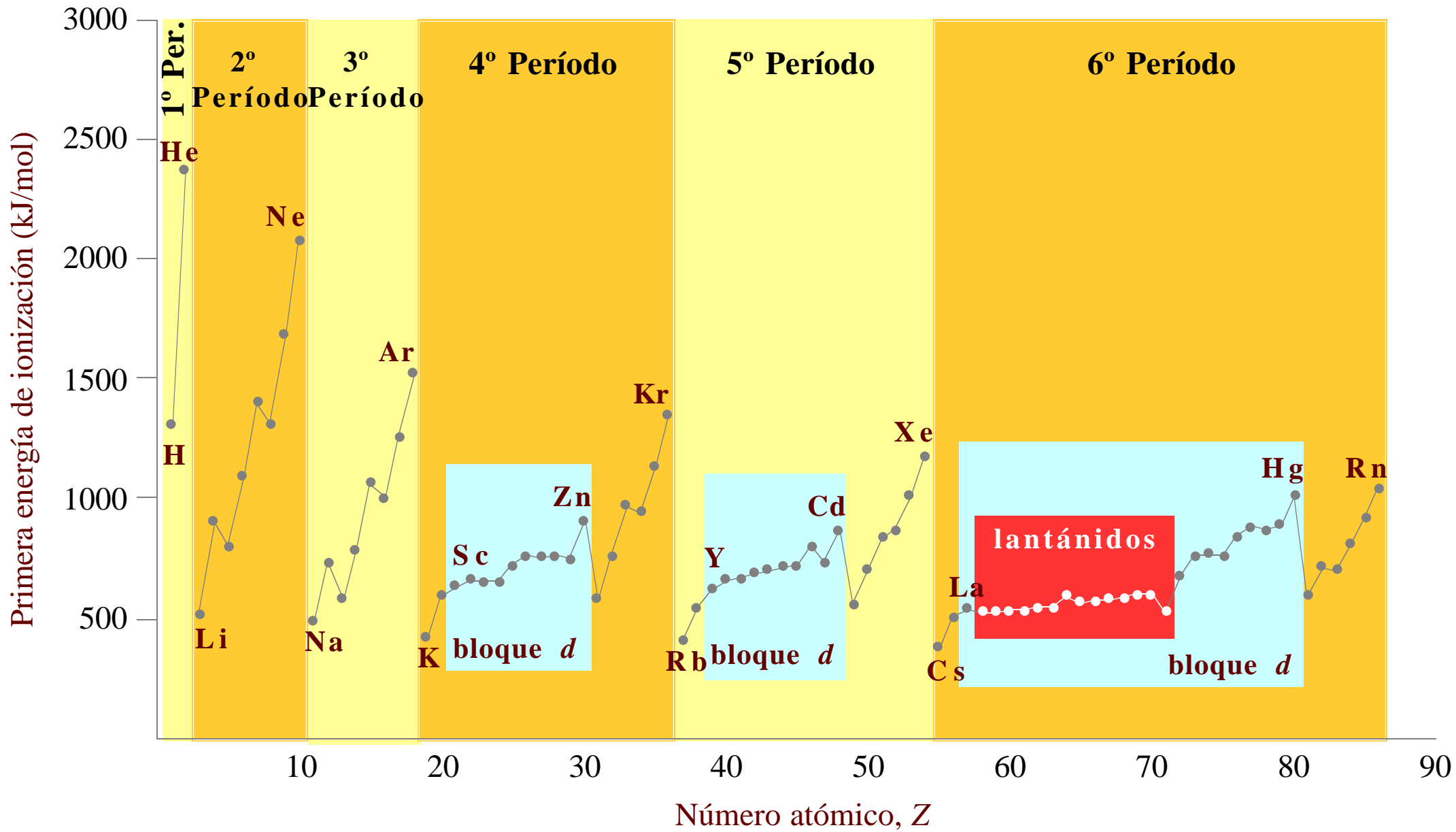






1Å





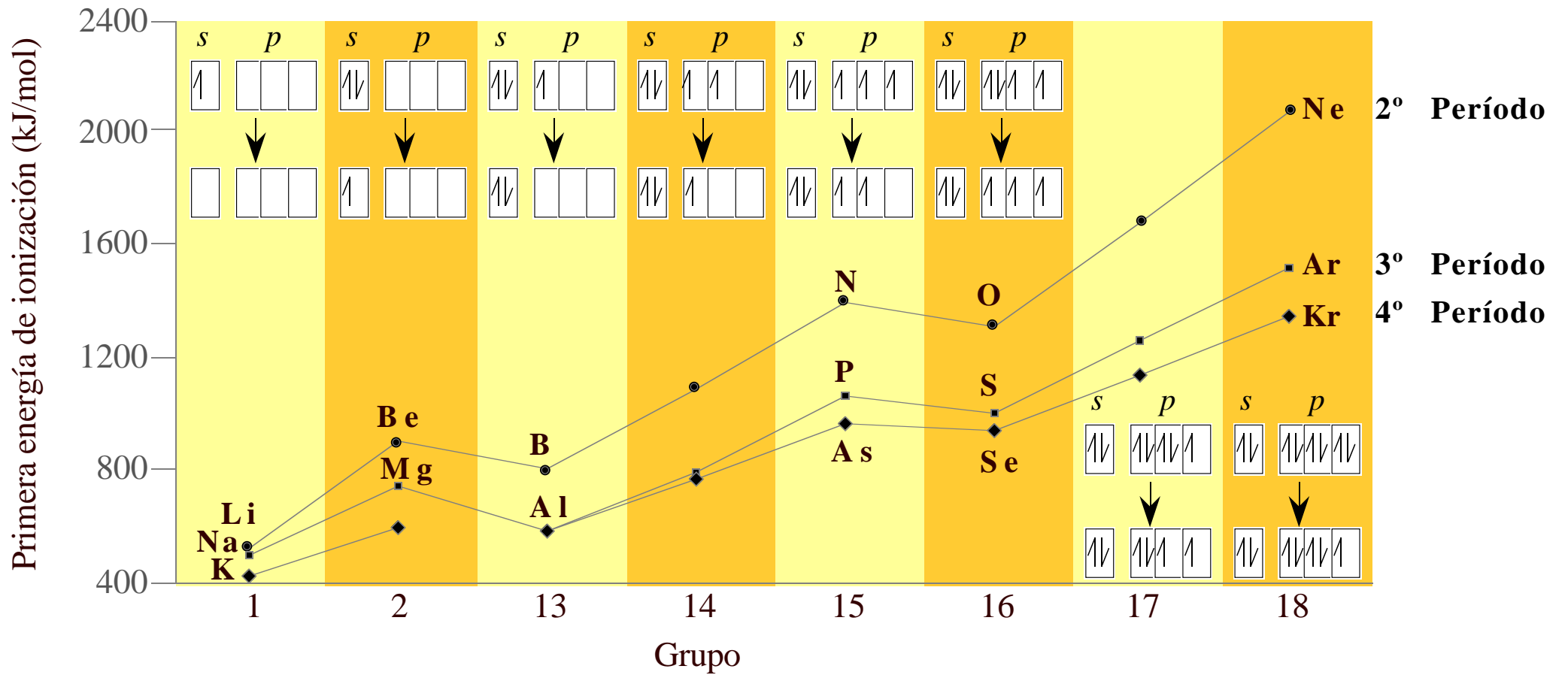








Tabla 1.11. Energías de ionización de los elementos del 2 al 5

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

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