A/Prof. Clemens ULRICH

Wed.	16:00 - 17:00	Old Main Building 149
Friday	9:00 - 10:00	Macauley Theatre (Quad 1027)

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Office Hour:

Monday: 1.30 – 3.00 pm
Room: 138D

Outline

1. Introduction:

- Planck Radiation
- Bohr's Model of the Atom
- Photoelectric Effect
- Compton Effect
- Dual Nature of Light: Particle Wave Dualism
- The Particle Wave: de Broglie Wavelength
- Heisenberg Uncertainty Principle
- Probability Function

Outline

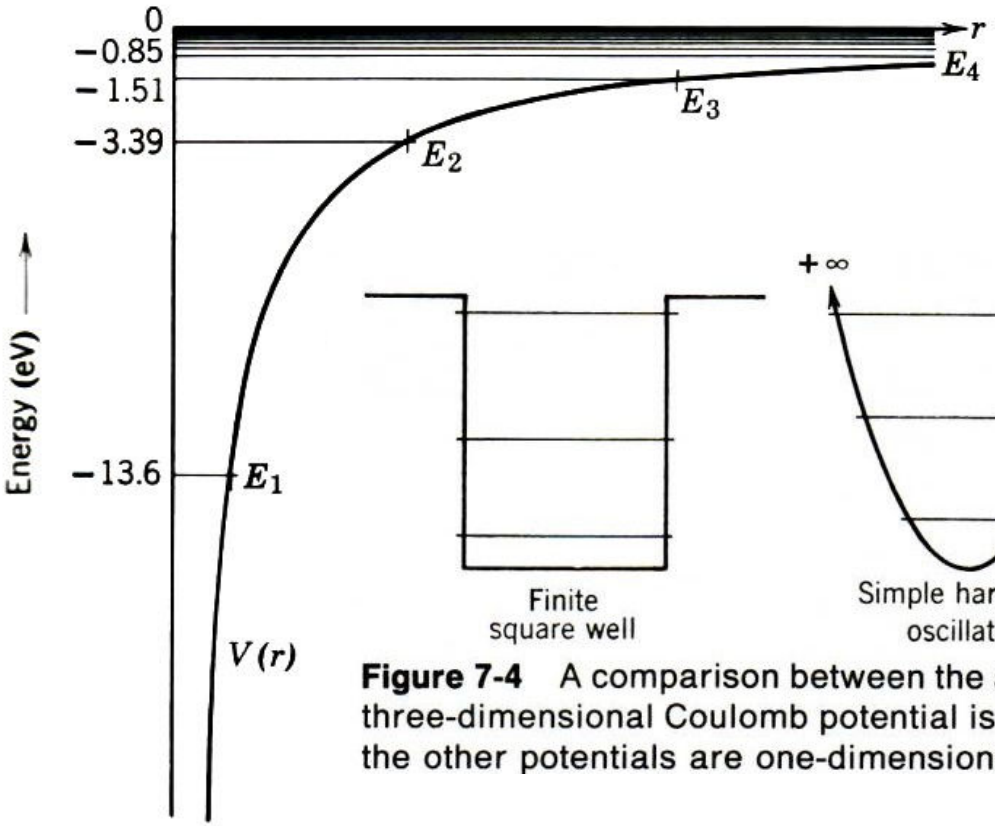
2. Quantum Theory of the free Particle:

- Schroedinger Equation of the free particle
- Time-independent Schroedinger Equation
- Eigenstate - Eigenfunction
- Particle in a box
- Linear quantum well
- The Harmonic Oscillator
- Quantum-mechanic Tunneling

Outline

3. Atomic Wavewfunctions:

- Schroedinger Equation of the Hydrogen Atom
- Atomic wavefunctions
- Separation of the angular and radial part
- Orbitals
- Angular momentum and spin
- Quantum numbers: **n, l, m, s**
- Hydrogen atom in a magnetic field
- Pauli principle: periodic table of elements



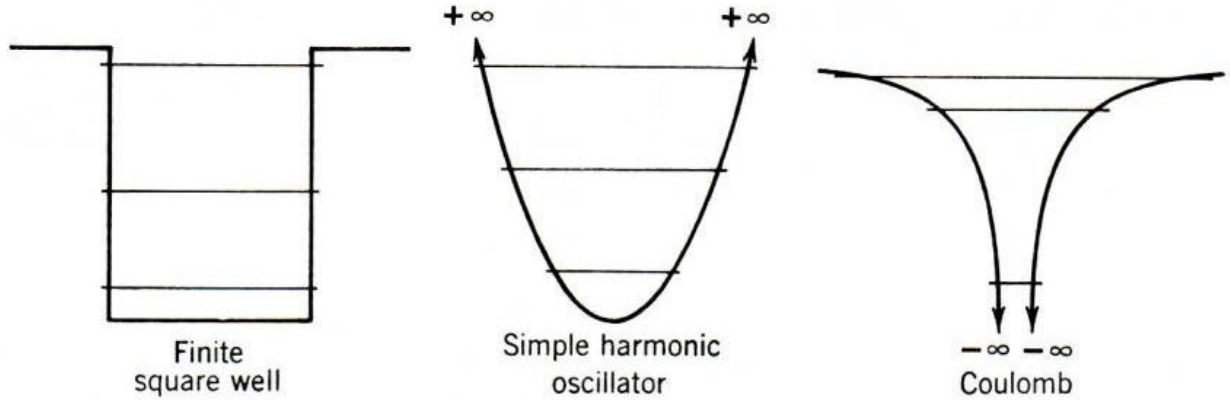


Figure 7-4 A comparison between the allowed energies of several binding potentials. The three-dimensional Coulomb potential is shown in a cross-sectional view along a diameter; the other potentials are one-dimensional.

Figure 7-3 The Coulomb potential $V(r)$ and its eigenvalues E_n. For large values of n the eigenvalues become very closely spaced in energy since E_n approaches zero as n approaches infinity. Note that the intersection of $V(r)$ and E_n, which defines the location of one end of the classically allowed region, moves out as n increases. Not shown in this figure is the continuum of eigenvalues at positive energies corresponding to unbound states.

from Eisberg/Resnick

$$R_{n,l}(r) = e^{-Zr/na_0}\left(\frac{Zr}{a_0}\right)^l G_{nl}\left(\frac{Zr}{a_0}\right)$$

Table 8.4 The Radial Wavefunctions $R_{n\ell}(r)$ of Hydrogen-like Atoms for n = 1, 2, and 3

n	ℓ	$R_{n\ell}(r)$
1	0	$\left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0}$
2	0	$\left(\frac{Z}{2a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
2	1	$\left(\frac{Z}{2a_0}\right)^{3/2}\frac{Zr}{\sqrt{3}\,a_0}e^{-Zr/2a_0}$
3	0	$\left(\frac{Z}{3a_0}\right)^{3/2} 2\left[1-\frac{2Zr}{3a_0}+\frac{2}{27}\left(\frac{Zr}{a_0}\right)^2\right]e^{-Zr/3a_0}$
3	1	$\left(\frac{Z}{3a_0}\right)^{3/2}\frac{4\sqrt{2}}{3}\frac{Zr}{a_0}\left(1-\frac{Zr}{6a_0}\right)e^{-Zr/3a_0}$
3	2	$\left(\frac{Z}{3a_0}\right)^{3/2}\frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

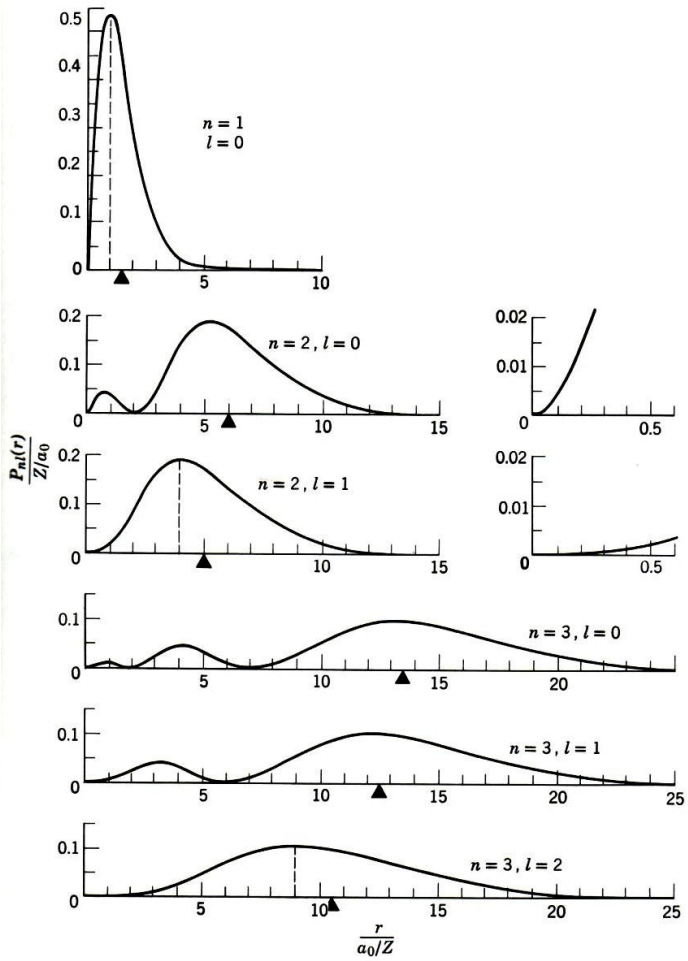


Figure 7-5 The radial probability density for the electron in a one-electron atom for n = 1, 2, 3 and the values of l shown. The triangle on each abscissa indicates the value of $\overline{r_{nl}}$ as given by (7-29). For $n = 2$ the plots are redrawn with abscissa and ordinate scales expanded by a factor of 10 to show the behavior of $P_{nl}(r)$ near the origin. Note that in the three cases for which $l = l_{max} = n - 1$ the maximum of $P_{nl}(r)$ occurs at $r_{Bohr} = n^2a_0/Z$, which is indicated by the location of the dashed line.

$$-\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\phi}\right)+\frac{m_l^{\,2}\Theta}{\sin^2\theta}=l(l+1)\Theta$$

Table 8.2 Some Associated Legendre Polynomials $P_\ell^{m_\ell}(\cos\theta)$

$P_0^0 = 1$
$P_1^0 = 2\cos\theta$
$P_1^1 = \sin\theta$
$P_2^0 = 4(3\cos^2\theta - 1)$
$P_2^1 = 4\sin\theta\cos\theta$
$P_2^2 = \sin^2\theta$
$P_3^0 = 24(5\cos^3\theta - 3\cos\theta)$
$P_3^1 = 6\sin\theta(5\cos^2\theta - 1)$
$P_3^2 = 6\sin^2\theta\cos\theta$
$P_3^3 = \sin^3\theta$

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi) = R_{n,l}(r)Y_{l,m_l}(\theta,\phi)$$

Table 7.2 Normalized Spherical Harmonics $Y(\theta, \phi)$

ℓ	m_ℓ	$Y_{\ell m_\ell}$
0	0	$\frac{1}{2\sqrt{\pi}}$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$
1	± 1	$\mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{\pm i\phi}$
2	0	$\frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$
2	± 1	$\mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$
2	± 2	$\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{\pm 2i\phi}$
3	0	$\frac{1}{4}\sqrt{\frac{7}{\pi}}(5\cos^3\theta - 3\cos\theta)$
3	± 1	$\mp\frac{1}{8}\sqrt{\frac{21}{\pi}}\sin\theta(5\cos^2\theta - 1)\, e^{\pm i\phi}$
3	± 2	$\frac{1}{4}\sqrt{\frac{105}{2\pi}}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
3	± 3	$\mp\frac{1}{8}\sqrt{\frac{35}{\pi}}\sin^3\theta\, e^{\pm 3i\phi}$

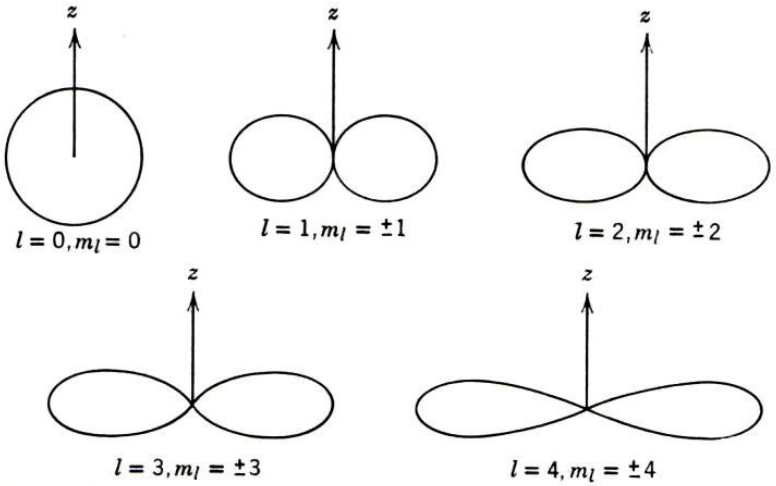


Figure 7-9 Polar diagrams of the directional dependence of the one-electron probability densities for $l = 0, 1, 2, 3, 4$; $m_l = \pm l$.

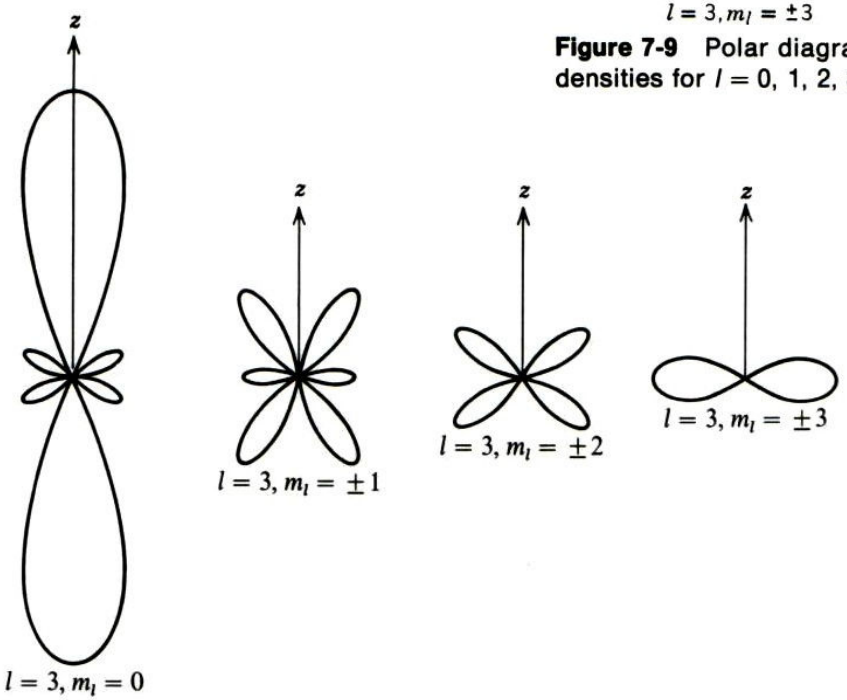
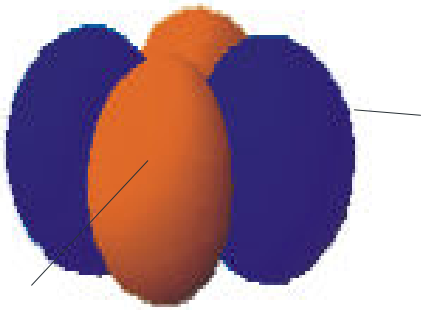
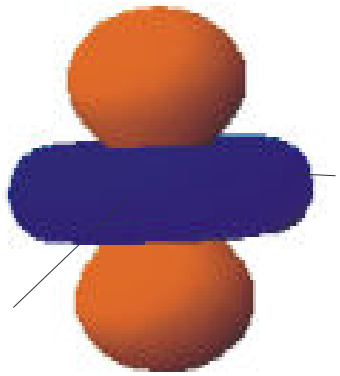


Figure 7-8 Polar diagrams of the directional dependence of the one-electron atom probability densities for $l = 3$; $m_l = 0, \pm 1, \pm 2, \pm 3$.

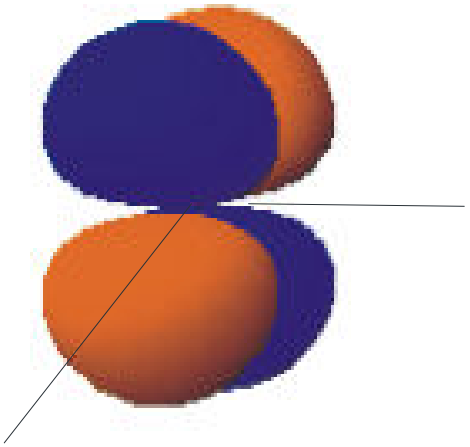
d-orbitals



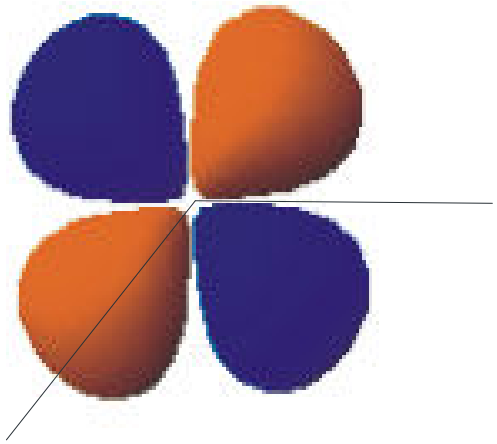
x^2-y^2



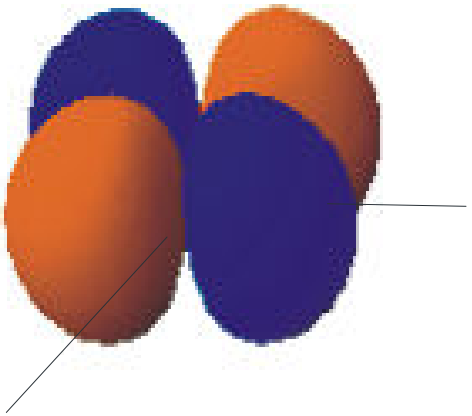
$3z^2$-r^2



xy

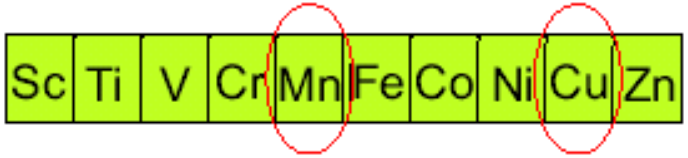


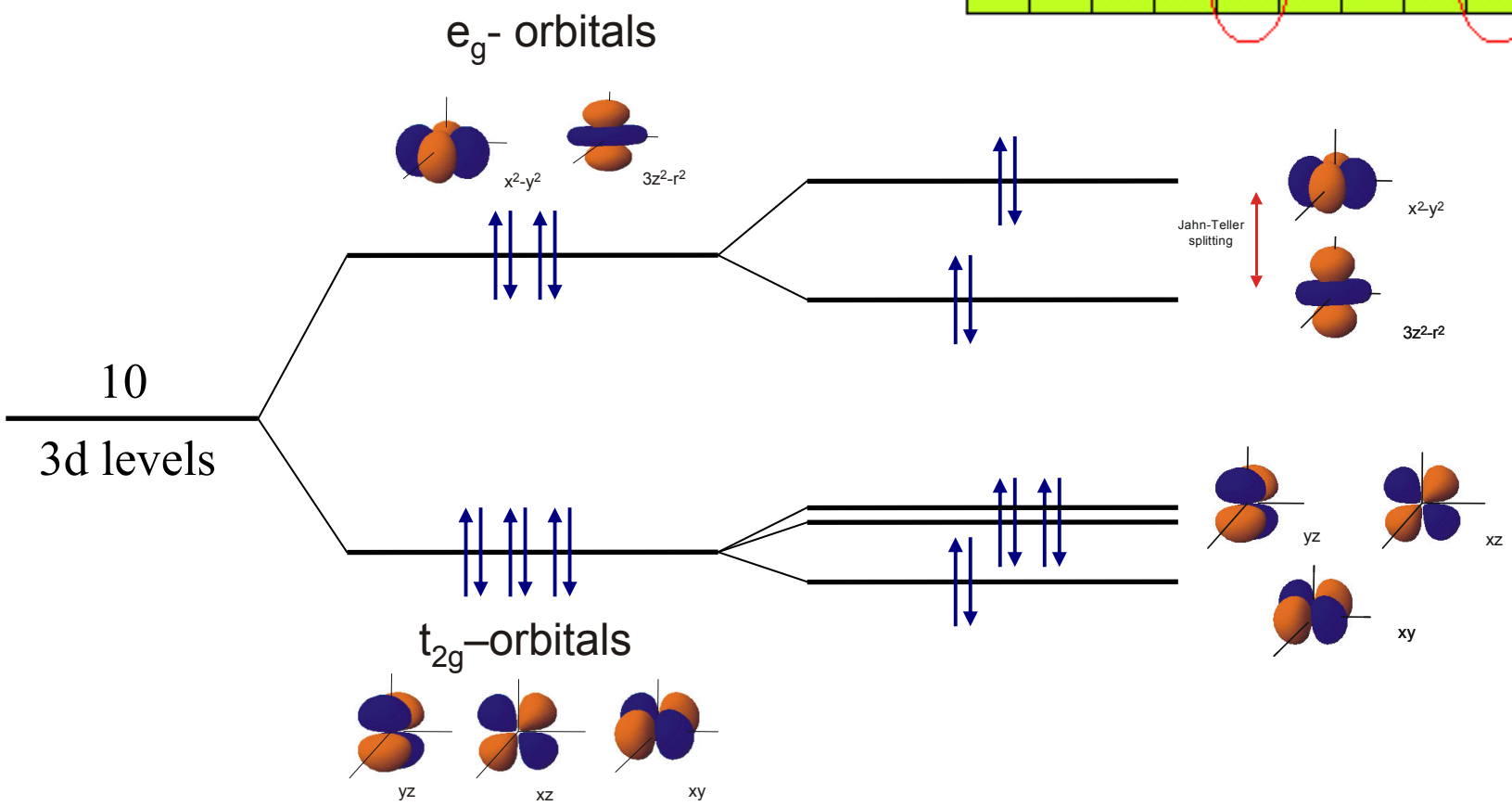
yz

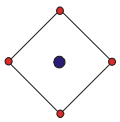


zx

Crystal Field Splitting of the 3d levels

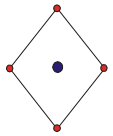




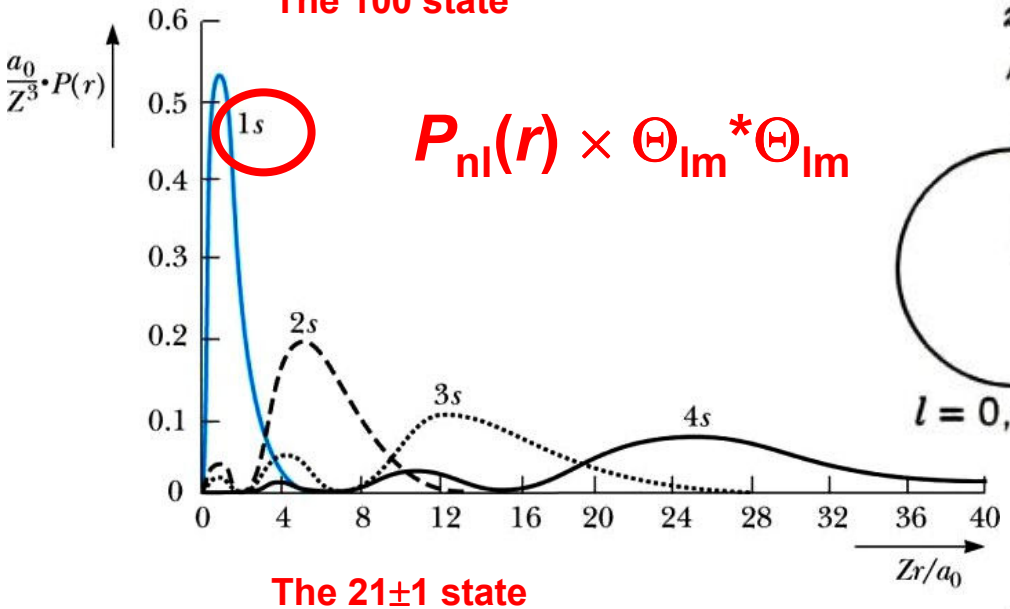


cubic splitting (octahedral)

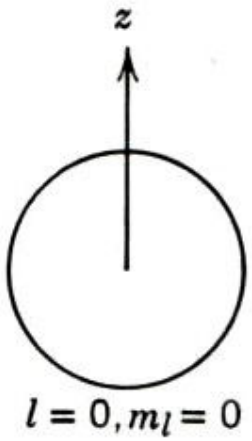
tetragonal splitting



The 100 state



$$P_{nl}(r) \times \Theta_{lm}^{*}\Theta_{lm}$$



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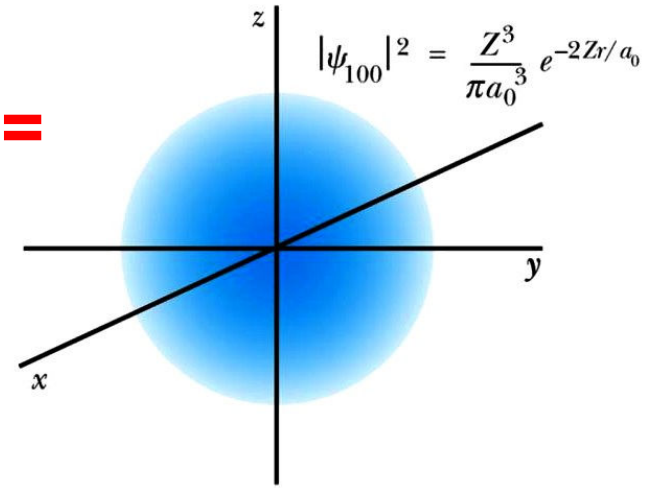
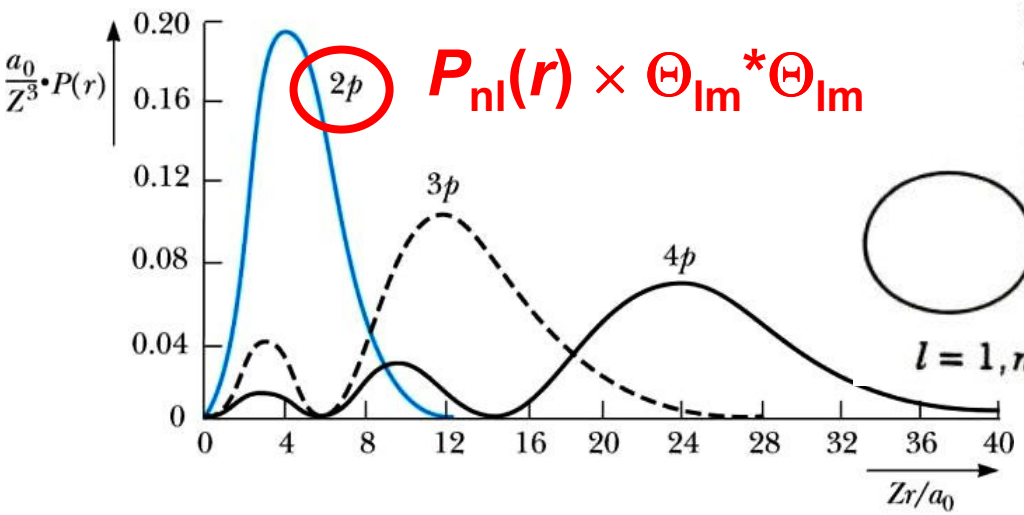
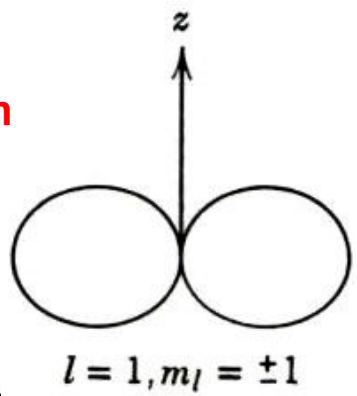


The 21±1 state



$$P_{nl}(r) \times \Theta_{lm}^{*}\Theta_{lm}$$



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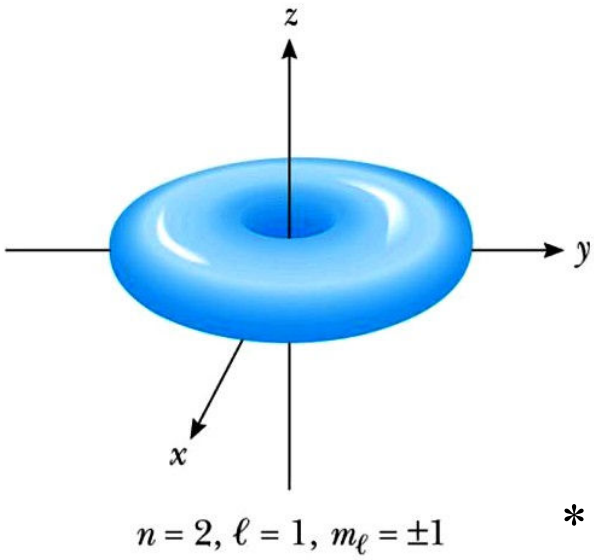

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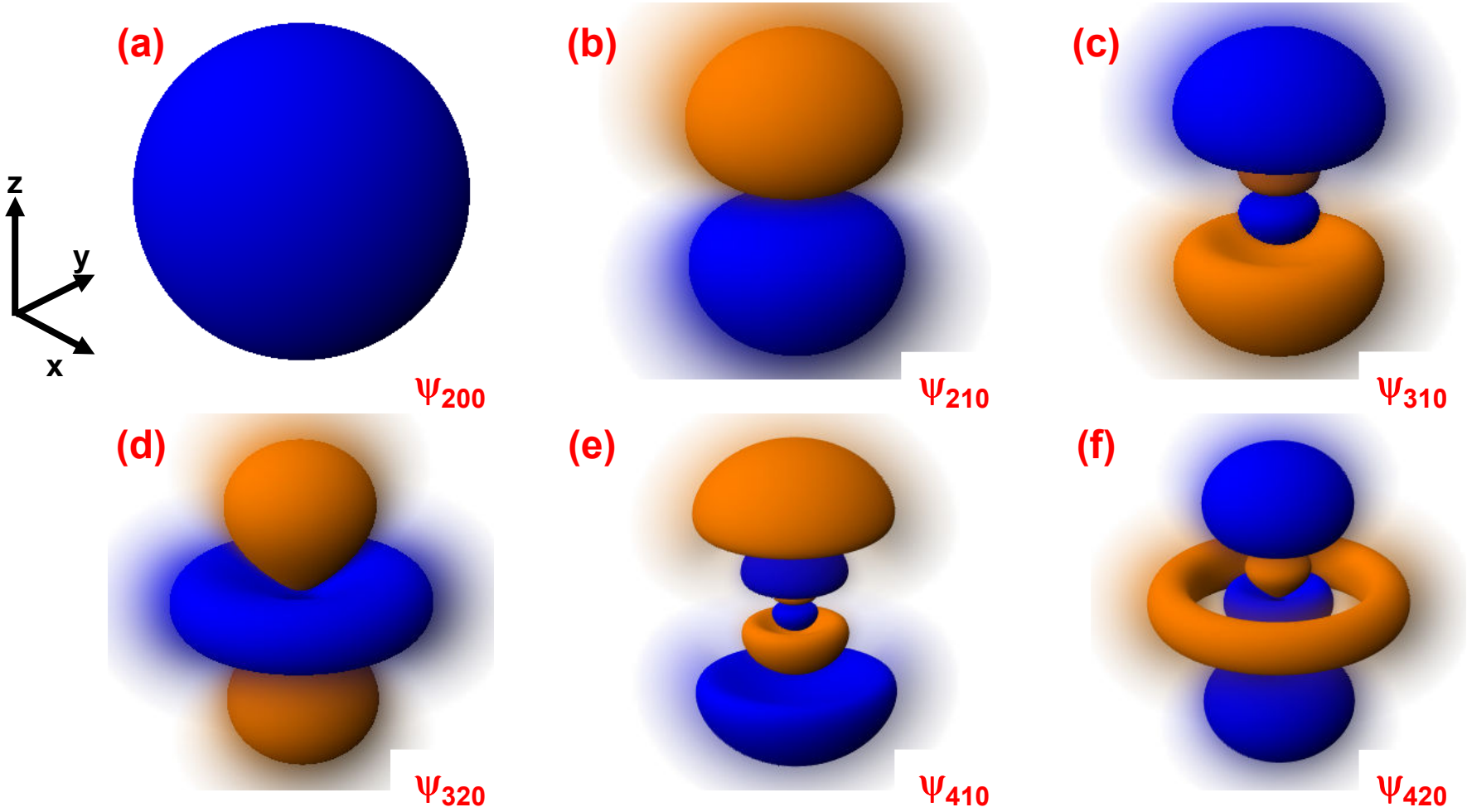
(a)
z
y
x
Ψ_{200}
(b)
Ψ_{210}
(c)
Ψ_{310}
(d)
Ψ_{320}
(e)
Ψ_{410}
(f)
Ψ_{420}

Wolfgang Pauli in 1925 (Nobel Prize 1945)

The exclusion principle states that no two electrons in an atom can have the same set of quantum numbers.

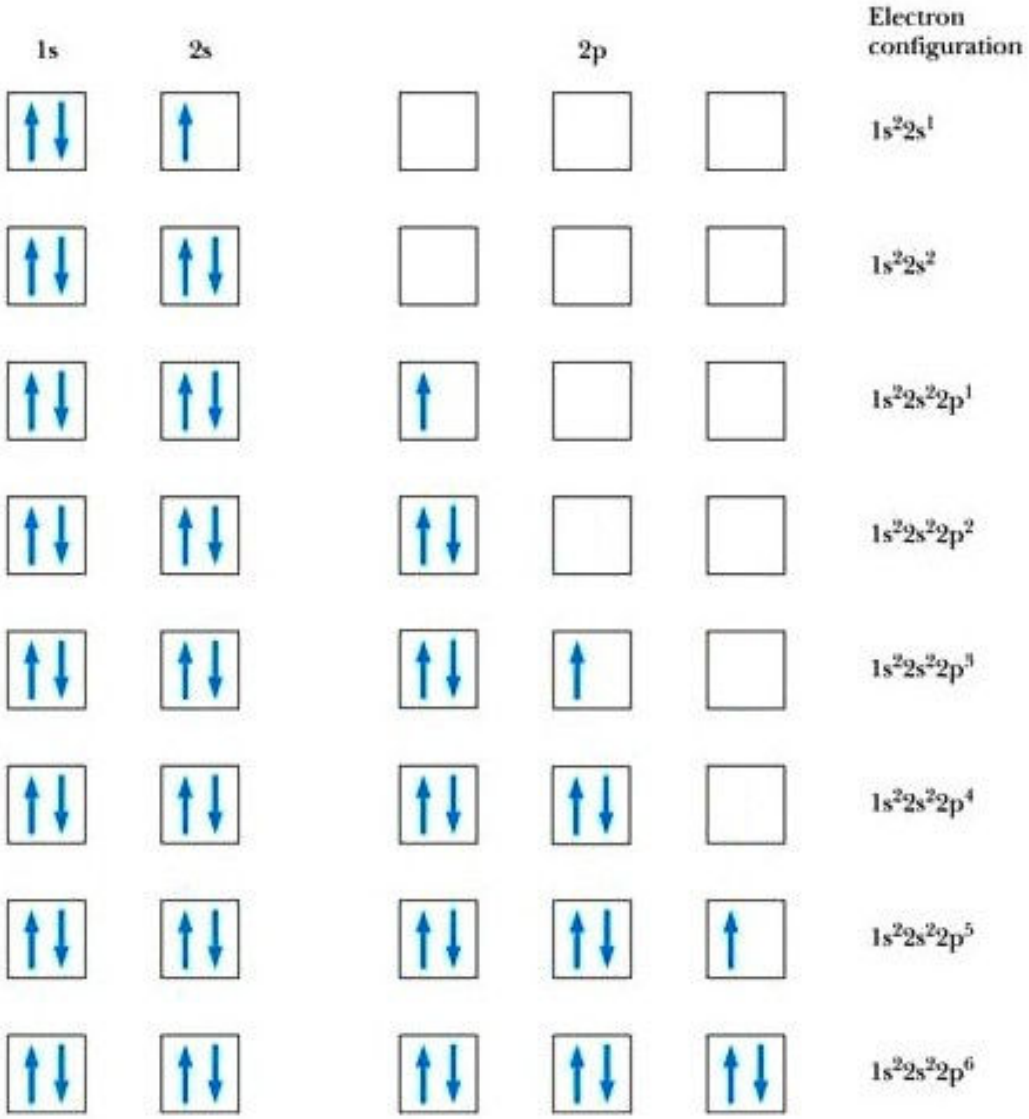

Table 9.2 Electronic Configurations of the Elements

Z	Symbol	Ground Configuration	Ionization Energy (eV)	Z	Symbol	Ground Configuration	Ionization Energy (eV)
1	H	$1s^1$	13.595	27	Co	$3d^7 4s^2$	7.86
2	He	$1s^2$	24.581	28	Ni	$3d^8 4s^2$	7.633
3	Li	[He] $2s^1$	5.390	29	Cu	$3d^{10} 4s^1$	7.724
4	Be	$2s^2$	9.320	30	Zn	$3d^{10} 4s^2$	9.391
5	B	$2s^2 2p^1$	8.296	31	Ga	$3d^{10} 4s^2 4p^1$	6.00
6	C	$2s^2 2p^2$	11.256	32	Ge	$3d^{10} 4s^2 4p^2$	7.88
7	N	$2s^2 2p^3$	14.545	33	As	$3d^{10} 4s^2 4p^3$	9.81
8	O	$2s^2 2p^4$	13.614	34	Se	$3d^{10} 4s^2 4p^4$	9.75
9	F	$2s^2 2p^5$	17.418	35	Br	$3d^{10} 4s^2 4p^5$	11.84
10	Ne	$2s^2 2p^6$	21.559	36	Kr	$3d^{10} 4s^2 4p^6$	13.996
11	Na	[Ne] $3s^1$	5.138	37	Rb	[Kr] $5s^1$	4.176
12	Mg	$3s^2$	7.644	38	Sr	$5s^2$	5.692
13	Al	$3s^2 3p^1$	5.984	39	Y	$4d 5s^2$	6.377
14	Si	$3s^2 3p^2$	8.149	40	Zr	$4d^2 5s^2$	6.835
15	P	$3s^2 3p^3$	10.484	41	Nb	$4d^4 5s^1$	6.881
16	S	$3s^2 3p^4$	10.357	42	Mo	$4d^5 5s^1$	7.10
17	Cl	$3s^2 3p^5$	13.01	43	Tc	$4d^5 5s^2$	7.228
18	Ar	$3s^2 3p^6$	15.755	44	Ru	$4d^7 5s^1$	7.365
19	K	[Ar] $4s^1$	4.339	45	Rh	$4d^8 5s^1$	7.461
20	Ca	$4s^2$	6.111	46	Pd	$4d^{10}$	8.33
21	Sc	$3d 4s^2$	6.54	47	Ag	$4d^{10} 5s^1$	7.574
22	Ti	$3d^2 4s^2$	6.83	48	Cd	$4d^{10} 5s^2$	8.991
23	V	$3d^3 4s^2$	6.74	49	In	$4d^{10} 5s^2 5p^1$	5.785
24	Cr	$3d^5 4s$	6.76	50	Sn	$4d^{10} 5s^2 5p^2$	7.342
25	Mn	$3d^5 4s^2$	7.432	51	Sb	$4d^{10} 5s^2 5p^3$	8.639
26	Fe	$3d^6 4s^2$	7.87	52	Te	$4d^{10} 5s^2 5p^4$	9.01

Table 9.2 Electronic Configurations of the Elements

Z	Symbol	Ground Configuration	Ionization Energy (eV)	Z	Symbol	Ground Configuration	Ionization Energy (eV)
53	I	$4d^{10}5s^25p^5$	10.454	79	Au	$[\mathrm{Xe}, 4f^{14}5d^{10}]\ 6s^1$	9.22
54	Xe	$4d^{10}5s^25p^6$	12.127	80	Hg	$6s^2$	10.434
55	Cs	$[\mathrm{Xe}]\ 6s^1$	3.893	81	Tl	$6s^26p^1$	6.106
56	Ba	$6s^2$	5.210	82	Pb	$6s^26p^2$	7.415
57	La	$5d6s^2$	5.61	83	Bi	$6s^26p^3$	7.287
58	Ce	$4f5d6s^2$	6.54	84	Po	$6s^26p^4$	8.43
59	Pr	$4f^36s^2$	5.48	85	At	$6s^26p^5$	9.54
60	Nd	$4f^46s^2$	5.51	86	Rn	$6s^26p^6$	10.745
61	Pm	$4f^56s^2$	5.60	87	Fr	$[\mathrm{Rn}]\ 7s^1$	3.94
62	Fm	$4f^66s^2$	5.644	88	Ra	$7s^2$	5.277
63	Eu	$4f^76s^2$	5.67	89	Ac	$6d7s^2$	5.17
64	Gd	$4f^75d6s^2$	6.16	90	Th	$6d^27s^2$	6.08
65	Tb	$4f^96s^2$	6.74	91	Pa	$5f^26d7s^2$	5.89
66	Dy	$4f^{10}6s^2$	6.82	92	U	$5f^36d7s^2$	6.194
67	Ho	$4f^{11}6s^2$	6.022	93	Np	$5f^46d7s^2$	6.266
68	Er	$4f^{12}6s^2$	6.108	94	Pu	$5f^67s^2$	6.061
69	Tm	$4f^{13}6s^2$	6.185	95	Am	$5f^77s^2$	5.99
70	Yb	$4f^{14}6s^2$	6.22	96	Cm	$5f^76d7s^2$	6.02
71	Lu	$4f^{14}5d6s^2$	6.15	97	Bk	$5f^86d7s^2$	6.23
72	Hf	$4f^{14}5d^26s^2$	6.83	98	Cf	$5f^{10}7s^2$	6.30
73	Ta	$4f^{14}5d^36s^2$	7.88	99	Es	$5f^{11}7s^2$	6.42
74	W	$4f^{14}5d^46s^2$	7.98	100	Fm	$5f^{12}7s^1$	6.50
75	Re	$4f^{14}5d^56s^2$	7.87	101	Mv	$5f^{13}7s^2$	6.58
76	Os	$4f^{14}5d^66s^2$	8.71	102	No	$5f^{14}7s^2$	6.65
77	Ir	$4f^{14}5d^76s^2$	9.12	103	Lw	$5f^{14}6d7s^2$	
78	Pt	$4f^{14}5d^86s^2$	8.88	104	Ku	$5f^{14}6d^27s^2$	

Periodensystem der Elemente

Ordungszahl — 6
Elementsymbol — C
Elementname — Kohlenstoff
Rel. Atommasse — 12.01

Fe — Feste Elemente
O — Gasförmige Elemente
Hg — Flüssige Elemente (20°C)
Tc — Radioaktive Elemente

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Wasserstoff 1.01																	2 He Helium 4.00
2	3 Li Lithium 6.94	4 Be Beryllium 9.01											5 B Bor 10.81	6 C Kohlenstoff 12.01	7 N Stickstoff 14.01	8 O Sauerstoff 15.999	9 F Fluor 18.998	10 Ne Neon 20.18
3	11 Na Natrium 22.99	12 Mg Magnesium 24.31											13 Al Aluminium 26.98	14 Si Silicium 28.09	15 P Phosphor 30.97	16 S Schwefel 32.07	17 Cl Chlor 35.45	18 Ar Argon 39.95
4	19 K Kalium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titan 47.88	23 V Vanadium 50.94	24 Cr Chrom 52.00	25 Mn Mangan 54.94	26 Fe Eisen 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.70	29 Cu Kupfer 63.55	30 Zn Zink 65.41	31 Ga Gallium 69.72	32 Ge Germanium 72.64	33 As Arsen 74.92	34 Se Selen 78.96	35 Br Brom 79.90	36 Kr Krypton 83.80
5	37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdän 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silber 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Zinn 118.71	51 Sb Antimon 121.76	52 Te Tellur 127.60	53 I Iod 126.90	54 Xe Xenon 131.29
6	55 Cs Cäsium 132.91	56 Ba Barium 137.33	La-Lu	72 Hf Hafnium 178.49	73 Ta Tantal 180.95	74 W Wolfram 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platin 195.08	79 Au Gold 196.97	80 Hg Quecksilber 200.59	81 Tl Thallium 204.38	82 Pb Blei 207.2	83 Bi Bismut 208.98	84 Po Polonium (209)	85 At Astat (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium (226)	Ac-Lr	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (262)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Ds Darmstadtium (281)	111 Rg Röntgenium (272)							

57 La Lanthan 138.91	58 Ce Cer 140.12	59 Pr Praseodym 140.91	60 Nd Neodym 144.24	61 Pm Promethium (147)	62 Sm Samarium 150.36	63 Eu Europium 151.97	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.97
89 Ac Actinium 227.03	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uran 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)