(3) **Today**

2.2 The Schrödinger Equation

2.2.1: The Particle in a Box

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

Next Class (4)

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

2.3 Periodic Properties

(5) **Second Class from Today**

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

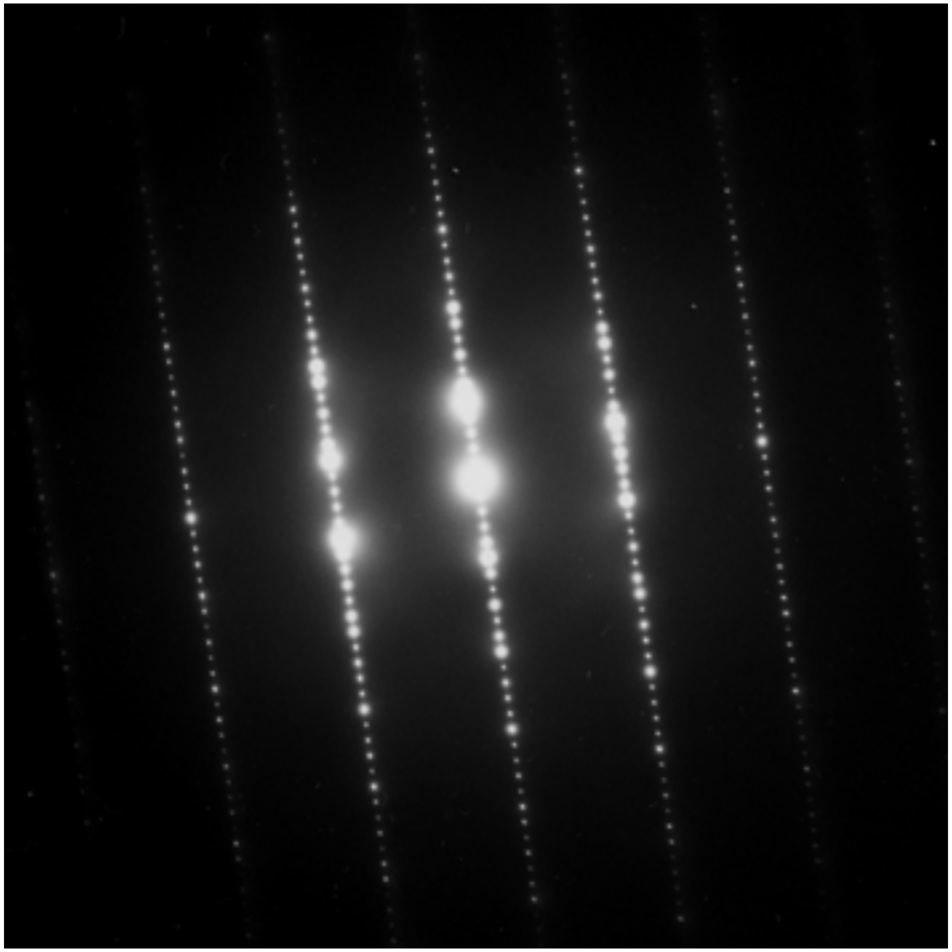
2.3 Periodic Properties

Third Class from Today (6)

3.1 Lewis Structures

3.2 VSEPR

Wave-Particle Duality



de Broglie $\lambda = h/\mathrm{mv}$

e^- have wavelike character

$\lambda = \frac{h}{mv}$ $\frac{\text{a tiny number}}{m_e \quad v_{e^-}}$ = λ is measureable

tiny # depends

Heisenberg $\Delta x \, \Delta p_x \geq h/4\pi$

$\lambda = \frac{h}{mv}$ $\frac{\text{tiny \#}}{\text{big \#}}$ = super tiny

people

https://en.wikipedia.org/wiki/Electron_diffraction#/media/File:DifraccionElectronesMET.jpg electron diffraction image obtained in a JEOL 2000FX TEM

Hamiltonian

$$H\Psi = E\Psi$$

wave function of the atom (linear combinations of the x of all the e^-'s)

Squaring the wave function gives use the probability of finding a the electron at a given location in space

The wave function must be an eigenfunction

wave functions are chosen base on mathematical knowledge or intuition

Necessary qualities of a wave function	
1. The wave function must be single valued.	Cannot have two probabilities for finding the electron at a given point
2. The wave function and its first derivatives must be continuous.	The probability must be defined at all points in space and cannot change abruptly
3. The wave function must approach 0 as r approaches infinity	The probability must get smaller at large distances of the atom. The atom must be finite.
4. Integrating $\Psi_A\Psi_A^*$ over all space must equal 1	The electron must be somewhere in space. Process is called normalizing the wave function
5. Integrating $\Psi_A\Psi_B^*$ over all space must equal 0	The orbitals must be orthogonal (mutually exclusive)

$$E = KE + PE$$

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0\sqrt{x^2 + y^2 + z^2}}$$

$$E = \frac{1}{2}mv^2 + \frac{kZq_1q_2}{r}$$

Since,

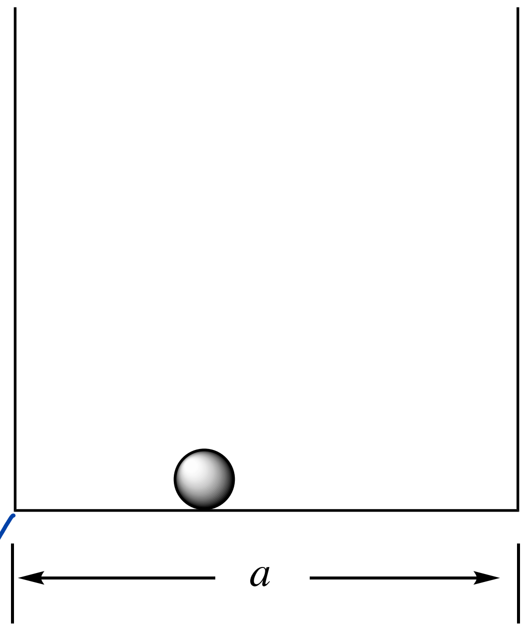
$$r = \sqrt{x^2 + y^2 + z^2}$$

KE

PE

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



0 probability

$$\Psi = \mathbf{A \sin rx + B \cos sx}$$

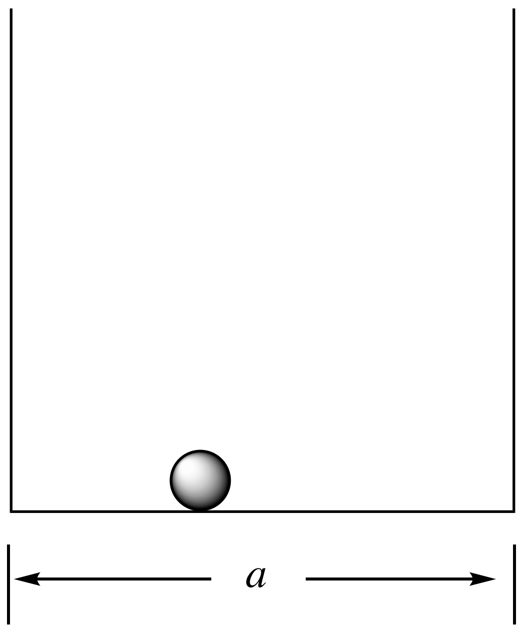
problem… if $x = 0$

$\cos s(0) = 1$

B must be 0

$$\Psi = \mathbf{A \sin rx}$$

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



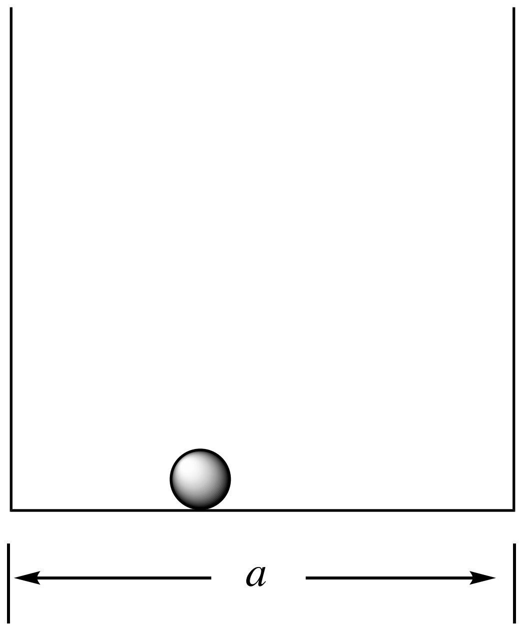
$$\Psi = \mathbf{A\ sin\ rx}$$

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \cancel{\frac{\delta^2}{\delta y^2}} + \cancel{\frac{\delta^2}{\delta z^2}}\right) - \cancel{\frac{Ze^2}{4\pi\varepsilon_0 r}}$$

H Ψ E ψ

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2}\left(A \sin rx\right)\right) = E\left(A \sin rx\right)$$

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box

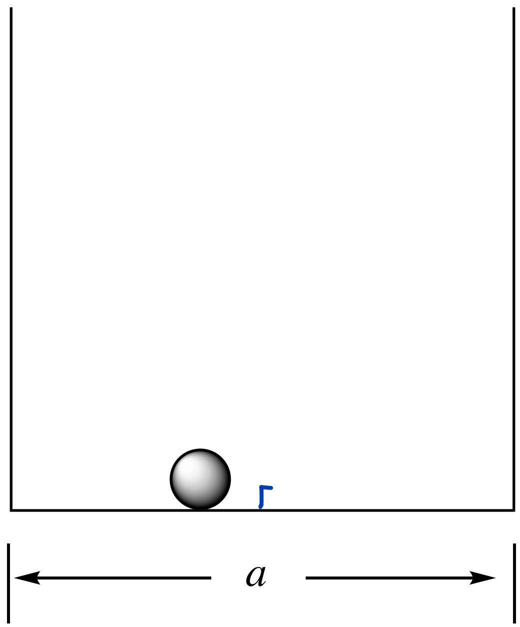


$$\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2}\left(A \sin rx\right)\right) = E\left(A \sin rx\right)$$

$$\frac{-h^2}{8\pi^2 m}\;(\;Ar)\left(\frac{\delta}{\delta x}\left(\cos rx\right)\right) = E\left(A \sin rx\right)$$

$$\frac{-h^2}{8\pi^2 m}\;(-Ar^2)\;(\sin rx) = E\;\;A \sin rx$$

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



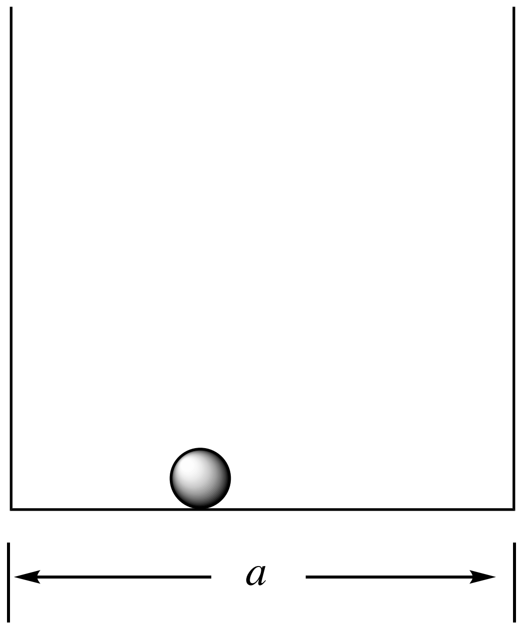
$$\frac{-h^2}{8\pi^2 m}(-\cancel{A}r^2)\cancel{(\sin rx)} = E\ \cancel{A \sin rx}$$

$$\frac{-h^2}{8\pi^2 m}(-r^2) = E$$

$$r^2 = E\,\frac{8\pi^2 m}{h^2}$$

$$r = \frac{2\pi}{h}\sqrt{2mE}$$

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



$$r = \frac{2\pi}{h}\sqrt{2mE}$$

But remember $\Psi = A \sin rx$

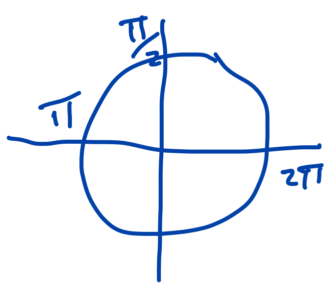
r must also equal $n\dfrac{\pi}{a}$

counting #

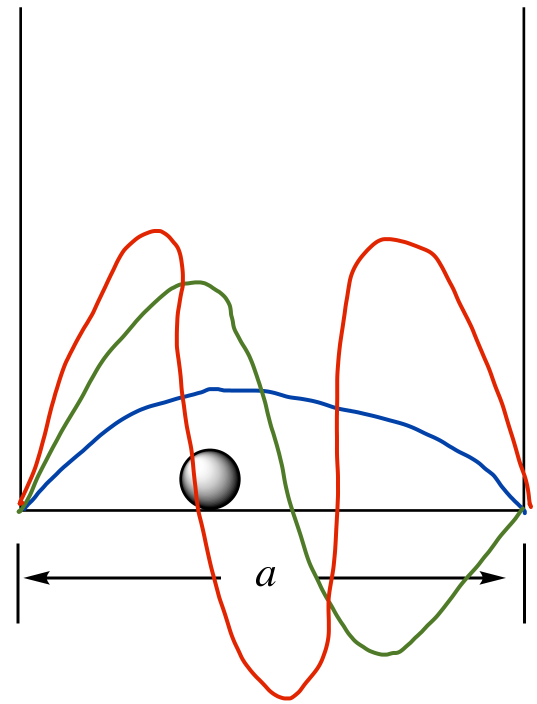
$\frac{\pi}{a} \times a = \pi$

So,

$$E = \frac{n^2h^2}{(8a^2m)}$$



So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



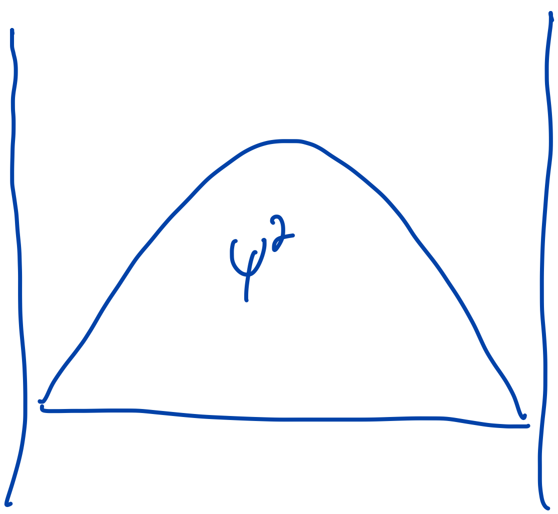
$$\Psi = \mathbf{A} \sin \mathbf{rx}$$

$$r = n\frac{\pi}{a}$$

$$\Psi = \mathbf{A} \sin(n\frac{\pi}{a}\,\mathbf{x})$$

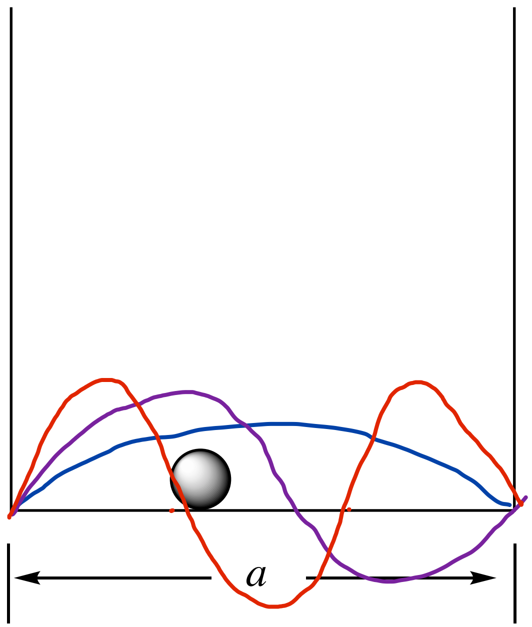
normalize the wave function

$A\int_{-\infty}^{\infty} \psi^*\psi = 1$ in this case, "all space" is from $x=0$ to $x=a$



lowest energy state we are most likely to find the ball in the middle of the box

So the electron is a particle/wave trapped in an atom…
Like a particle trapped in a box



$$\Psi = \mathbf{A}\ \mathbf{sin}(\,n\frac{\pi}{a}\ \mathbf{x})$$

$$(\Psi\Psi^*) = 1$$

$$\boldsymbol{\Psi} = (2/a)^{1/2}\ \mathbf{sin}\ (n\pi/a)\mathbf{x}$$

excited states

n=1 n=2 n=3

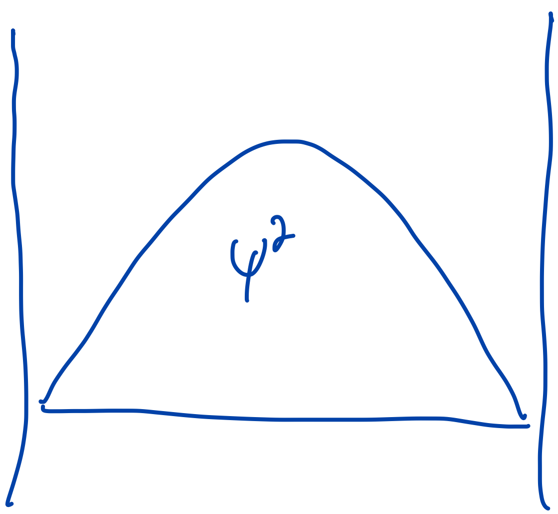
ground state for particle

in its lowest energy state

we are most likely to find

the ball in the middle of

the box



Equations

https://www.westfield.ma.edu/cmasi/advinorg/angular_distribution_functions/text_and_graphics_containe.htm

Pictures

https://www.westfield.ma.edu/cmasi/advinorg/quant_orbital_surfaces/orbital_surfaces.htm

Models

s and p

https://www.westfield.ma.edu/cmasi/organic/mo-plain/aos.html

d orbitals

https://www.westfield.ma.edu/cmasi/advinorg/dorbs/dorbsp.html

One quantum number wasn't enough to model the electrons in an atom

n is the principal quantum number

allowed values are the whole numbers starting a 1

l is the Angular momentum quantum number

allowed values are the from ~~n~~ $n-1$ to 0 in whole number increments

m_l is the magnetic quantum number

allowed values are the from $-l$ to *l* in whole number increments

m_s is the spin quantum number

allowed values are $-\,^1/_2$ or $+^1/_2$

The angular distribution function:
The square of the angular distribution function describes the probability of finding the electron at angles θ and ϕ.
In other words, picture yourself standing on the nucleus, and the electrons look like fog around you. The square of the angular distribution function describes how thick fog is when you look in different directions.
The Angular distribution function describes the basic shape of the orbital, or the number of nodal planes in an orbital.
The angular distribution functions depend only on the quantum numbers ***l*** and $\mathbf{m_l}$. That is, the angular distribution functions of all electrons with the same ***l*** and $\mathbf{m_l}$ values are the same regardless of **n** or $\mathbf{m_s}$. Another way of saying this is that all s orbitals have the same basic shape. For example The 2s orbital (n = 2, *l* = 0, m_l = 0), the 3s (n = 3, *l* = 0, m_l = 0) and the 4s (n = , *l* = 0, m_l = 0) have the same basic shape; they are all spherically symmetrical.

The radial distribution function:
The square of the radial distribution function describes the probability of finding an a electron a given distance from the nucleus.
In other words, it tells you how far away the fog starts to tapper off, and it tells you whether or not there are pockets of clear sky in the fog.
The radial distribution function describes how far away from the nucleus the orbital extends and the number of nodal surfaces the orbital has.
The radial distribution functions depend on **both n** and ***l***. This means that the number of nodal surfaces and an orbital has and how far that orbital extends from the nucleus depends on the principle quantum number or energy level of the orbital (the **1** in **1**s, the **2** in **2**s, the **3** in **3**s, etc.) and the type of orbital (s vs. p vs. d ***l*** = 0, 1, or 2).

ℓ is the orbital type. $\ell = 0$ is an s orbital

no angular dependence for the wave function

Quantum Numbers	Angular Distribution Function	Radial Distribution Function
$n = 1, \ell = 0$	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(1s) = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{(-\sigma)}$ ← probability falls to 0 at ∞
$n = 2, \ell = 0$ s	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(2s) = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}(2-\sigma)\, e^{\left(-\frac{\sigma}{2}\right)}$ probability falls to 0 at $\sigma = 2$
$n = 3, \ell = 0$	$\chi(s) = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$	$R(3s) = \frac{2}{81\sqrt{3}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}(27 - 18\sigma + 2\sigma^2)\, e^{\left(-\frac{\sigma}{3}\right)}$
$n = 2, \ell = 1$ p	$\chi(P_x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \sin\theta \cdot \cos\phi$ $\chi(P_y) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \sin\theta \cdot \sin\phi$ $\chi(P_z) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \cos\theta$	$R(2p) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\sigma\, e^{\left(-\frac{\sigma}{2}\right)}$

$\sigma = Zr/a_0$ $a_0 = \varepsilon_0 h^2/(\pi e^2 m_e)$

Principles of Mordern Chemistry, 2nd edition. Oxtoby, D.W.; Nachtrieb, N. H. Saunders College Publishing, 1990.

periodic table is shaped by quantum mechanics

The so called families of elements react similarly because, as quantum mechanics tell us, they have similar arrangements of electrons in their highest energy orbitals

Periodic Table of the Elements

	1	2															3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																															2 He
2	3 Li	4 Be																									5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg																									13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca															21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr															39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

$n=3$

$n=4$

$n=4$

$n=5$

s f d p

all halogens are $ns^2 np^5$

https://en.wikipedia.org/wiki/Periodic_table