9.1 Atomic Physics. II

Quantum numbers

Pauli Exclusion Principle

Periodic Table

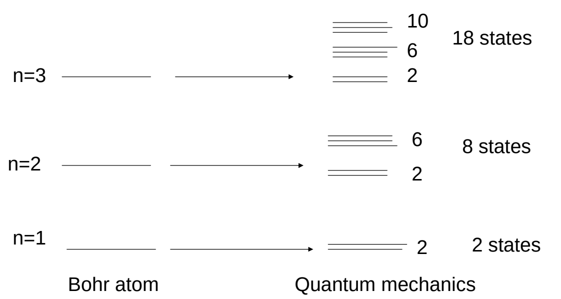
Characteristic x-rays

Electrons in atoms.

Electrons in atoms exist in discrete energy levels which can be calculated by solving a wave equation. This calculation is beyond the scope of this course.

However, the pattern of energy levels which results from a quantum mechanical rule called the Pauli Exclusion Principle. is responsible for the periodicity in the chemical properties of the different elements as seen in the Periodic Table.

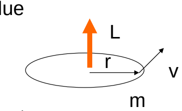
Quantum calculations show that more states are needed to describe the electrons in an atom



The number of states determined by quantum numbers.

Orbital angular momentum

Classically the angular momentum L of an electron moving in a circle can have any value

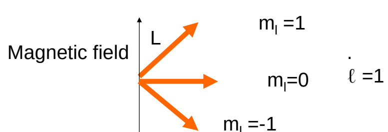


In quantum mechanics the values of the angular momentum are quantized and specified by a orbital angular momentum quantum no. ℓ

For an electron with a principle quantum no. n the value of ℓ ranges from 0 to n-1.

i.e. for n=2 , ℓ can have values of 0 and 1.

Orbital magnetic quantum number



Classically an electron moving in a circle is a current which results in a magnetic dipole.

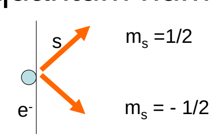
Classically, the dipole can have any orientation with respect to a field.

In quantum mechanics, only discrete orientations are allowed. The orientation are determined by the orbital magnetic quantum no. m_l

The value of m_l ranges from – ℓ to + ℓ.

i.e. for ℓ=1, m_l can have values of -1, 0, and 1.

Spin magnetic quantum number



In quantum mechanics an electron has an intrinsic magnetic moment due to spin. The magnetic moment can have two orientations in a magnetic field determined by a spin quantum number m_s

m_s = +1/2 or -1/2

for an electron 2 spin states are possible $\pm$ 1/2

Atomic energy levels and quantum numbers.

	range of values
principle quantum number n	1, 2, 3, ...
angular momentum quantum number ℓ	0, 1 to n-1
orbital magnetic quantum number m_ℓ	$-\ell,..\text{to}..+\ell$
spin magnetic quantum number m_s	$-\frac{1}{2},\text{or}+\frac{1}{2}$

The state of an electron is specified by the set of its quantum numbers (n, ℓ, m_l, m_s)
The number of states is determined by the set of possible quantum numbers.

Electronic states in an atom n=1,2 and 3

n	l	m_l	m_s	no. of states	no. n, l	no. n
1	0	0	±½	2	2	2
2	0	0	±½	2	2	8
2	1	-1	±½	2	6	
2	1	0	±½	2		
2	1	1	±½	2		
3	0	0	±½	2	2	18
3	1	-1	±½	2	6	
3	1	0	±½	2		
3	1	1	±½	2		
3	2	-2	±½	2	10	
3	2	-1	±½	2		
3	2	0	±½	2		
3	2	1	±½	2		
3	2	2	±½	2		

Pauli Exclusion Principle

No two electrons in an atom can have the same quantum number, n, l, m_l, or m_s.

To form an atom with many electrons the electrons go into the lowest energy unoccupied state.

The periodic properties of the elements as shown in the Periodic Table can be explained by the Pauli Exclusion Principle by properties of filled shells.

Electrons in atoms- Shell Notation

TABLE 28.1

Shell and Subshell Notation

n	Shell Symbol	ℓ	Subshell Symbol
1	K	0	s
2	L	1	p
3	M	2	d
4	N	3	f
5	O	4	g
6	P	5	h
...		...	

TABLE 28.3

Number of Electrons in Filled Subshells and Shells

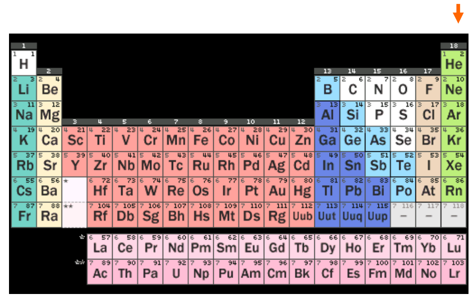
Shell	Subshell	Number of Electrons in Filled Subshell	Number of Electrons in Filled Shell
K ($n = 1$)	$s(\ell = 0)$	2	2
L ($n = 2$)	$s(\ell = 0)$	2	8
	$p(\ell = 1)$	6	
M ($n = 3$)	$s(\ell = 0)$	2	18
	$p(\ell = 1)$	6	
	$d(\ell = 2)$	10	
N ($n = 4$)	$s(\ell = 0)$	2	32
	$p(\ell = 1)$	6	
	$d(\ell = 2)$	10	
	$f(\ell = 3)$	14	

Periodic Table of the Elements

Dmitri Mendeleev (1834-1907)

noble gases

Z



2
10
18
36
54
86

Noble gas configurations

Noble gases have Filled Subshells

He Z= 2 $1s^2$

Ne Z=10 $1s^2$ $2s^2$ $2p^6$

Ar Z=18 $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$

Kr Z= 36 $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ $4s^2$ $4p^6$

Noble gases have filled subshells

Stable, difficult to ionize $A \rightarrow A^+ + e^-$

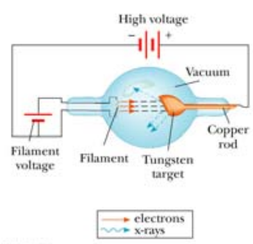
TABLE 28.4

Electronic Configurations of Some Elements

Z	Symbol	Ground-State Configuration	Ionization Energy (eV)	Z	Symbol	Ground-State Configuration	Ionization Energy (eV)
1	H	$1s^1$	13.595	19	K	[Ar] $4s^1$	4.339
2	He	$1s^2$	24.581	20	Ca	$4s^2$	6.111
				21	Sc	$3d4s^2$	6.54
3	Li	[He] $2s^1$	5.390	22	Ti	$3d^24s^2$	6.83
4	Be	$2s^2$	9.320	23	V	$3d^34s^2$	6.74
5	B	$2s^22p^1$	8.296	24	Cr	$3d^54s^1$	6.76
6	C	$2s^22p^2$	11.256	25	Mn	$3d^54s^2$	7.432
7	N	$2s^22p^3$	14.545	26	Fe	$3d^64s^2$	7.87
8	O	$2s^22p^4$	13.614	27	Co	$3d^74s^2$	7.86
9	F	$2s^22p^5$	17.418	28	Ni	$3d^84s^2$	7.633
10	Ne	$2s^22p^6$	21.559	29	Cu	$3d^{10}4s^1$	7.724
				30	Zn	$3d^{10}4s^2$	9.391
11	Na	[Ne] $3s^1$	5.138	31	Ga	$3d^{10}4s^24p^1$	6.00
12	Mg	$3s^2$	7.644	32	Ge	$3d^{10}4s^24p^2$	7.88
13	Al	$3s^23p^1$	5.984	33	As	$3d^{10}4s^24p^3$	9.81
14	Si	$3s^23p^2$	8.149	34	Se	$3d^{10}4s^24p^4$	9.75
15	P	$3s^23p^3$	10.484	35	Br	$3d^{10}4s^24p^5$	11.84
16	S	$3s^23p^4$	10.357	36	Kr	$3d^{10}4s^24p^6$	13.996
17	Cl	$3s^23p^5$	13.01				
18	Ar	$3s^23p^6$	15.755				

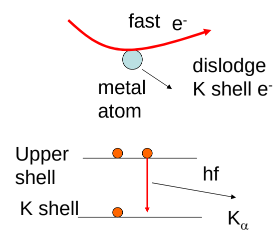
Filled subshell configuration s^2 , p^6 , d^{10}

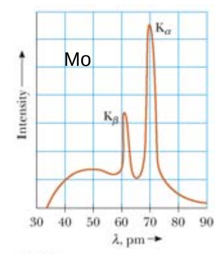
Characteristic X-rays are due to emission from heavy atoms excited by electrons



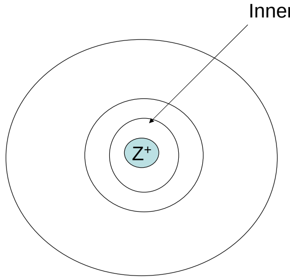
Characteristic x-rays

The wavelength of characteristic x-ray peaks due to emission from high energy states of heavy atoms (high Z).





A Bohr model for x-ray emission



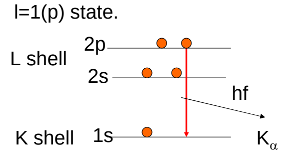
Energy from Bohr model

$$E_n = Z_{eff}^2(13.6)\frac{1}{n^2}$$

Z_{eff} is an effective charge of the nucleus due to screening.

X-ray emission

Calculate the wavelength for K_α x-ray emission of Mo (Z=+42). The electron in the L shell must come from a l=1(p) state.



L shell Z_{eff} =Z-3

K shell Z_{eff} = Z-1

$$E_{(Lshell)} = -13.6(Z-3)^2\left(\frac{1}{2^2}\right)$$

$$E_{Kshell} = -13.6(Z-1)^2\left(\frac{1}{1^2}\right)$$

$$\Delta E = 13.6(41)^2\left[\frac{1}{1}\right] - 13.6(39)^2\left[\frac{1}{4}\right] = 1.77x10^4 eV$$

$$\Delta E = hf = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.63x10^{-34}J)(3.0x10^8 m/s)}{(1.6x10^{-19}J/eV)(1.77x10^4 eV)} = 7.0x10^{-11}m$$

Comparison experiment

Calculated
value
70 pm