Unit 2: Chemical Bonding and Organic Chemistry

Chapter 7: Atomic Structure and Periodicity

7.1: Electromagnetic Radiation

Electromagnetic (EM) Radiation: - energy that travels at the speed of light in a form of perpendicular waves. This includes everything from cosmic rays to radio waves.

Wavelength (λ): - the length of a wave (from crest to crest).

Frequency (v): - the number of wave in one second; measures in Hertz (Hz) or s^{-1} . (1 Hz = 1 s^{-1})



EM Wave	Frequency (Hz)	Wavelength (m)	EM Wave	Frequency (Hz)	Wavelength (m)
Cosmic Wave	10^{23}	10^{-15}	Infrared	10^{12}	10^{-4}
Gamma Wave	10^{20}	10^{-12}	Microwaves	10^{10}	10^{-2}
X-Ray	10^{18}	10^{-10}	FM Radio	10^8 or (100 MHz)	1 to 10
Ultraviolet	10^{16}	10^{-8}	Shortwave Radio	10 ⁶ (1 MHz)	10^{2}
Visible	$(7.5 \text{ to } 4.3) \times 10^{14}$	$(4 \text{ to } 7) \times 10^{-7}$	AM Radio	$10^4 (10 \text{ kHz})$	10^{4}
	(blue to red)	400 nm to 700 nm			
		(blue to red)			

Example 1: One of the spectral lines of hydrogen has a wavelength of 410 nm. Determine the corresponding frequency.

$$c = 2.9979 \times 10^{8} \text{ m/s}$$

$$\lambda = 410 \text{ nm} = 410 \times 10^{-9} \text{ m}$$

$$v = ?$$

$$c = \lambda v$$

$$v = \frac{c}{\lambda} = \frac{(2.9979 \times 10^{8} \text{ m/s})}{(410 \times 10^{-9} \text{ m})}$$

$$v = 7.31 \times 10^{14} \text{ s}^{-1} \text{ (Hz)}$$

Example 2: What is the wavelength being broadcast by a radio station with a frequency of 102.1 MHz?

 $c = 2.9979 \times 10^{8} \text{ m/s} \qquad c = \lambda v$ $v = 102.1 \text{ MHz} = 102.1 \times 10^{6} \text{ s}^{-1} \qquad \lambda = \frac{c}{v} = \frac{(2.9979 \times 10^{8} \text{ m/s})}{(102.1 \times 10^{6} \text{ s}^{-1})} \qquad \lambda = 2.94 \text{ m}$

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7.2: The Nature of Matter

Photoelectric Effect: - Einstein's experiment with photoelectric tube found that electrons can only be emitted from a metal surface in a cathode ray tube when a threshold (minimum)

frequency is directed at it. (*Intensity or Brightness of the light is not a factor*) - the slope of amount of energy of the emitted electrons per frequency used is called the **Planck's constant** (h) = 6.626 × 10⁻³⁴ J s (in honour of Max Planck who first



Example 2: What is the minimum frequency needed if it takes 450 kJ to remove one mole of electrons from a metal surface of a photoelectric tube?

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$\Delta E_{\min} = W = -450 \text{ kJ/mol}$$
(negative because of energy input)
$$w_{\min} = ?$$

$$\Delta E_{\min} = -450 \times 10^{3} \text{ J/mol} \times \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ e}^{-}} = -7.47 \times 10^{-21} \text{ J}$$

$$w_{\min} = \frac{W}{-h} = \frac{(-7.47 \times 10^{-21} \text{ J})}{-(6.626 \times 10^{-34} \text{ J s})}$$

$$w_{\min} = 1.13 \times 10^{13} \text{ s}^{-1}$$

<u>Duality of Light</u>: - EM Radiation has characteristics of wave (reflection, refraction, and diffraction) and particles (momentum and kinetic energy as demonstrated by Einstein). These <u>light</u> particles are called photons.

- Photons have no mass. But its mass equivalence can be calculated as follows.

$$E = mc^{2}$$
 (Einstein's Mass Energy Conservation)

$$m = \frac{E}{c^{2}}$$

$$m = \frac{\left(\frac{hc}{\lambda}\right)}{c^{2}} = \frac{hc}{\lambda c^{2}}$$
 (Substitute $E = \frac{hc}{\lambda}$ and simplify)
Mass Equivalence of a Photon

$$m = \frac{h}{\lambda c}$$
 (*m* is in kg)

<u>de Broglie Wavelength</u>: - since light can behave like particles; particles can have wave properties. - rearranging the mass equivalence of a photon formula above and replacing c with speed of the actual particle (nothing that has mass can travel at the

speed of light – Einstein Theory of Relativity), we have the following

de Broglie Wavelength

$$\lambda = \frac{h}{mv}$$

$$v = \text{speed of particle (m/s)}$$

$$m = \text{mass of particle (kg)}$$

Example 3: Calculate the de Broglie wavelength of a proton with a mass of 1.67×10^{-27} kg moving at 25.0% of the speed of light.

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$\upsilon = 0.25 (2.9979 \times 10^8 \text{ m/s})$$

$$= 74,947,500 \text{ m/s}$$

$$m = 1.67 \times 10^{-27} \text{ kg}$$

$$\lambda = \frac{h}{m\upsilon} = \frac{(6.626 \times 10^{-34} \text{ J s})}{(1.67 \times 10^{-27} \text{ kg})(74947500 \text{ m/s})} \quad (1 \text{ J} = 1 \text{ kg m}^2/\text{s}^2)$$

$$\lambda = 5.29 \times 10^{-15} \text{ m}$$

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Example 4: What is the velocity of an alpha particle (2 protons) that has a wavelength of 3.30×10^{-14} m as it is travelling towards a piece of gold foil in the Rutherford experiment?

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$m = 2(1.67 \times 10^{-27} \text{ kg})$$

$$= 3.34 \times 10^{-27} \text{ kg}$$

$$\lambda = 3.30 \times 10^{-14} \text{ m}$$

$$\upsilon = \frac{h}{m\lambda} = \frac{(6.626 \times 10^{-34} \text{ J s})}{(3.34 \times 10^{-27} \text{ kg})(3.30 \times 10^{-14} \text{ m})} \quad (1 \text{ J} = 1 \text{ kg m}^2/\text{s}^2)$$

$$\upsilon = ?$$

$$\upsilon = 6.01 \times 10^6 \text{ m/s}$$

7.3: The Atomic Spectrum of Hydrogen

- **<u>Quantized Energy</u>**: because electrons can only exist at a particular orbital at one time, and never between orbitals, it can only emit a certain wavelength as it comes down from an excited state to the ground state.
- **<u>Diffraction</u>**: as wave encountered an opening (slit), its wavelength is separated into as the wave is scattered.
- **<u>Diffraction Pattern</u>**: the pattern of bright and dark spots due to the interference of the wave front because a wave has travelled through a slit.
- <u>Continuous Spectrum</u>: as white light travelled through a prism, it is diffracted and the visible light spectrum (red to violet) is observed.

Line Spectrum: - when light from an excitation of a particular atom, the quantized energy is emitted as specific wavelength as it travels from higher excited orbitals to the lower orbitals.



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7.4: The Bohr Model

Quantum Model: - proposed by Niels Bohr, electron in hydrogen atom moves around the nucleus in specific circular orbits, which have certain energies.

- Energy needs to be input ($\Delta E > 0$) to move up the orbitals.
- Energy is given off as frequency ($\Delta E < 0$) to move down the orbitals.

$$\boldsymbol{E}_{\boldsymbol{\infty}} = \mathbf{0} \mathbf{J} \quad \boldsymbol{n} = \boldsymbol{\infty}$$



Example 1: Verify that the blue line (434.0 nm) of the visible part of the hydrogen spectrum is indeed from the emission of energy of an electron moving from the 5th orbital to the 2nd orbital.

$$\Delta E = E_{f} - E_{i}$$

$$\Delta E = \frac{-2.178 \times 10^{-18} \text{ J}}{n_{f}^{2}} - \frac{-2.178 \times 10^{-18} \text{ J}}{n_{i}^{2}}$$

$$\Delta E = -2.178 \times 10^{-18} \text{ J} \left(\frac{1}{n_{f}^{2}} - \frac{1}{n_{i}^{2}}\right)$$

$$\Delta E_{5 \to 2} = -2.178 \times 10^{-18} \text{ J} \left(\frac{1}{2^{2}} - \frac{1}{5^{2}}\right)$$

$$\Delta E_{5 \to 2} = -4.5675 \times 10^{-19} \text{ J} \left(\Delta E < 0 \text{ means energy is released}\right)$$

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Example 2: Determine the ionization energy (from ground state to infinity) of hydrogen in J and in eV. Explain the meaning of the sign in the calculated value.

$$\Delta E = E_f - E_i$$

$$\Delta E = \frac{-2.178 \times 10^{-18} \text{ J}}{n_f^2} - \frac{-2.178 \times 10^{-18} \text{ J}}{n_i^2} = -2.178 \times 10^{-18} \text{ J} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$\Delta E_{1 \to \infty} = -2.178 \times 10^{-18} \text{ J} \left(\frac{1}{\infty^2} - \frac{1}{1^2}\right) \qquad \text{(Note: } \frac{1}{\infty^2} \approx 0\text{)}$$

$$\Delta E_{1 \to \infty} = -2.178 \times 10^{-18} \text{ J} \qquad (\Delta E > 0 \text{ means energy is absorbed)}$$

$$\Delta E_{1 \to \infty} = 2.178 \times 10^{-18} \text{ J} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \qquad \Delta E_{1 \to \infty} = 13.61 \text{ eV}$$

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7.5: The Quantum Mechanical Model of the Atom

Schrödinger Wave Equation:- Schrödinger recognized that since electron can behave like waves (de
Broglie), he proposed that electron can have quantized energy when it
achieved a standing wave (wave that appears standing because it contains
nodes which signifies exactly half a wavelength).Standing Wave
(2 nodes - 1 half- λ)Standing Wave
(3 nodes - 2 half- λ)Standing Wave
(4 nodes - 3 half- λ)

Schrödinger Wave Equation

 $\hat{H}\psi = E\psi$

 \hat{H} = Hamiltonian Operator (This is not a variable, but a combination of calculation procedures like integrals, $\int \psi(x, y, z) d(x, y, z)$, and derivatives $d\psi(x, y, z)/d(x, y, z)$.)

 ψ = Wave Function

E = Total Energy (Electric Potential and Kinetic Energies)

Note: If the wave function (ψ) remains the same after the operation by the Hamiltonian Operator (\hat{H}), then the coefficient of the final wave function is the total energy of the atom (E). The wave function can now be used to calculate the probability distribution of the electron around the nucleus.

<u>Heisenberg Uncertainty Principle</u>: - at very high velocity, we cannot know precisely the position and momentum (mass times velocity) of a particle at a given time.

Heisenberg Uncertainty Principle $\Delta x \bullet \Delta(m\upsilon) \ge \frac{h}{4\pi}$ $\Delta x = \text{Uncertainty in particle's position} \qquad \Delta(m\upsilon) = \text{Uncertainty in particle's momentum}$ As $\Delta x \downarrow$ (more certain in particle's position), $\Delta(m\upsilon) \uparrow$ (less certain in particle's momentum)

<u>Probability Distribution</u> (R^2) : - the probability of the likely position of an electron around a nucleus. - the probability distribution is equalled to the square of the wave function.

> Probability Distribution $R^{2} = \left[\psi(x, y, z)\right]^{2}$ $\psi(x, y, z) = \text{Wave Function in } x, y, \text{ and } z \text{ directions}$

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Electron Density (Probability) Map: - a diagram that shows the probability distribution of an electron around the nucleus; also called **atomic orbital**.



<u>Radial Probability Distribution</u>: - when total probability (Surface Area of a Sphere × Probability) is plotted against distance from the nucleus.

- at small radius, probability is big but surface area is small (yields low total probability).
- at large radius, probability is small but surface area is big (yields low total probability)
- at optimal radius, surface area × probability is large (maximum total probability = Atomic Radius).



7.6: Quantum Numbers

Quantum Numbers: - a series of number that demonstrates the properties of different atomic orbitals.

- a. <u>Principal Quantum Number</u> (*n*): natural number values {1, 2, 3, ...} are used to describe the energy and size of the orbital.
- **b.** <u>Angular Momentum Quantum Number</u> (ℓ): whole numbers $\{0 \le \ell \le (n-1)\}$ are used to indicate the shape of the atomic orbitals.

ℓ = 0 (s orbital) "sharp"	ℓ = 1 (p orbital) "principal"	ℓ = 2 (<i>d</i> orbital) "diffuse"	<pre>l = 3 (f orbital) "fundamental"</pre>	$\ell = 4$ (g orbital) (follows the alphabet after f)

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c. <u>Magnetic Quantum Number</u> (m_{ℓ}) : - integral numbers $\{-\ell \le m_{\ell} \le \ell\}$ are used to show the orientation of the orbital in space relative to the other orbitals in the atom.

- each m_{ℓ} value represents an atomic orbital.

Check out the websites at:

- 1. Schrödinger Equation in Three Dimensions: <u>http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/sch3d.html#c2</u>
- 2. Hydrogen Schrödinger Equation: <u>http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydsch.html#c1</u>
- <u>Subshell</u>: orbital designation as indicated by Principal Quantum Number (*n*) and the letter used for Angular Momentum Quantum Number (ℓ).

<u>n</u>	l	<u>Subshell</u>	<u>m</u> ,	Number of Orbitals	Total Number of Orbitals
1	0	1 <i>s</i>	0	1	1
2	0	2 <i>s</i>	0	1	4
	1	2 <i>p</i>	-1, 0, 1	3	4
3	0	3 <i>s</i>	0	1	
	1	3 <i>p</i>	-1, 0, 1	3	9
	2	3d	-2, -1, 0, 1, 2	5	
4	0	4 <i>s</i>	0	1	
	1	4p	-1, 0, 1	3	16
	2	4d	-2, -1, 0, 1, 2	5	16
	3	4 <i>f</i>	-3, -2, -1, 0, 1, 2, 3	7	
5	0	5 <i>s</i>	0	1	
	1	5 <i>p</i>	-1, 0, 1	3	
	2	5 <i>d</i>	-2, -1, 0, 1, 2	5	25
	3	5f	-3, -2, -1, 0, 1, 2, 3	7	
	4	5g	-4,-3, -2, -1, 0, 1, 2, 3, 4	9	

Example 1: Explain why the following sets of quantum numbers or subshells are incorrect.

a. 3*f*

n = 3 $\ell = 0, 1, \text{ or } 2$ (*s*, *p*, or *d* subshells) Since n = 3, we cannot have a *f* subshell.

n = 1 $\ell = 0$ (s subshell only) Since n = 1, we cannot have a d subshell.

<u>Assignment</u>
7.4 pg. 338 #51 to 58
7.5 pg. 339 #65
7.6 pg. 338 #61 to 64

b. $n = 3, \ell = 3, m_{\ell} = -2$

n = 3 $\ell = 0, 1, \text{ or } 2$ $m_{\ell} = -2, -1, 0, 1 \text{ or } 2$ Since n = 3, we cannot have a $\ell = 3$.

d. $n = 5, \ell = 4, m_{\ell} = 5$

n = 5 $\ell = 0, 1, 2, 3 \text{ or } 4$ $m_{\ell} = -4, -3, -2, -1, 0, 1, 2, 3 \text{ or } 4$

Since n = 5, and the maximum $\ell = 4$, we cannot have a $m_{\ell} = 5$.

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7.7: Orbital Shapes and Energies

<u>Orbital Shapes</u>: - from the Schrödinger wave functions, the graph the radial probability distributions in 3 dimensions forms the orbital shapes.

<u>Nodal Surfaces (Nodes)</u>: - the areas between orbitals where there is zero probability of electron distribution.





Degenerate: - in the case of hydrogen atom where orbitals of the same *n* value shares the same energy level.



7.8: Electron Spin and the Pauli Principle

Electron Spin: - when electron spins clockwise, it creates a magnetic north pole in the upward direction. Conversely, when electron spins counter-clockwise, it creates a magnetic north pole in the downward direction.



<u>Electron Spin Quantum Number</u> (m_s) : - values of $\pm \frac{1}{2}$ to denote the electron spin direction.

<u>Pauli Exclusion Principle</u>: - in a given atom, no two electrons can have exactly the same set of four quantum numbers $(n, \ell, m_{\ell}, \text{ and } m_{s})$.

- an orbital can only hold two electrons with opposing spins.

Example 1: In the 1*s* orbital, the four quantum numbers for the two electrons are:



7.9: Polyelectronic Atoms

Polyelectronic Atoms: - atoms with more than one electron (all non-hydrogen atoms).

<u>Electron Correction Problem</u>: - due to the mathematical difficulty in calculating the repulsion of electrons in polyelectronic atoms (since Heisenberg Uncertainty Principle rules out predicting the exact location and momentum of an electron), an assumption needs to be made that the valence electrons are "screened" or "shielded" from the <u>nuclear charge</u> which composes of the inner electrons and the protons in the nucleus.

Penetration (Tunnelling) Effect: - the result where electrons in higher s or p orbitals have a other

maximum radial probabilities in closer proximity to the nucleus than d orbital at the same energy level.



Check out the websites at:

- 1. Electron Configurations: http://intro.chem.okstate.edu/WorkshopFolder/Electronconfnew.html
- 2. Whizzy Periodic Table: http://www.colorado.edu/physics/2000/applets/a2.html

<u>Assignment</u> 7.7 pg. 339 #67 and 68 7.8 pg. 339 #69 and 79

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7.10: The History of the Periodic Table

Johann Dobereiner: - first to discover a pattern of a group of elements like Cl, Br, and I (called triads).

- John Newland: suggested elements should be arranged in "octaves" because they repeat their properties for every eighth elements.
- **Dmitri Mendeleev**: conceived the first modern periodic table of elements. (independently worked on by Julius Lothar Meyer).
 - insisted certain spots of the table be left blank until the actual element is found that matched the predicted properties. This was done to preserve the elements with similar properties called groups or families.

7.11: The Aufbau Principle and the Periodic Table

Aufbau Principle: - "Aufbau" German for "building up"

- for each element, electrons are added up into the hydrogen like quantum orbitals as protons are being added to the nucleus.

Orbital Diagram: - a diagram that shows the arrangements of electrons in quantum subshells.

<u>Hund's Rule</u>: - for subshells that can have more than 1 orbital (as in p, d, f...), the lowest energy can be achieved when the electrons are arranged so that there are a maximum number of unpaired electrons. These unpaired electrons are drawn "spinning up" (\uparrow) in the orbital diagram.

Electron Configuration: - the arrangement of electrons in atomic subshells.

	1 1		· · · · · ·	1	4	1 1	1.	1		41	1 /	C.		C	41	C 11	•	4	
Hyami	ne i	•	iraw t	ne ai	llannim	ornital	diagram	ເຈກດ	CTATE	The	electron	CONTI	ouratior	ic tor	The	TOUM	owinc	r_{atom}	с.
Плаш	JICI	L. D	marr i	no qu	uantum	oronar	ulagram	s and	state	unc		comi	guianoi	10 101	unc	IOII	0 w mg	atom	э.
							0						9				6	,	

Atomic #	Atom	Electron Configuration	Orbital Diagram
1	Н	1 <i>s</i> ¹	$\uparrow \qquad \qquad$
2	Не	$1s^2$	↓
3	Li	$1s^2 2s^1$	↑↓ ↑
4	Be	$1s^2 2s^2$	
5	В	$1s^2 2s^2 2p^1$	↑↓ ↑↓ ↑
6	C	$1s^2 2s^2 2p^2$	↑↓ ↑↓ ↑ ← ─
7	N	$1s^2 2s^2 2p^3$	↑↓ ↑↓ ↑- ↑- ↑-
8	0	$1s^2 2s^2 2p^4$	<u>↑↓</u> ↑↓ ↑↓ ↑→
9	F	$1s^2 2s^2 2p^5$	
10	Ne	$1s^2 2s^2 2p^6$	

<u>Core Electrons</u>: - inner electrons that have completed a row in the Periodic Table of Elements.

Valance Electrons: - electrons in the outermost principal quantum number of an atom.

- elements in the same group or family contains the same valence electron configuration.

Example 2: Draw the quantum orbital diagrams and state the electron configurations for the following atoms.

Atomic #	Atom	Electron Configuration	Orbital Diagram
	¹ ttom	Electron Conngulation	4s 3d 4p
19	Κ	$[\mathbf{Ar}] \ 4s^1$	[Ar] 1
20	Ca	$[\mathbf{Ar}] \ 4s^2$	[Ar] 🛧
21	Sc	[Ar] $4s^2 3d^1$	[Ar] + +
22	Ti	$[\mathbf{Ar}] \ 4s^2 \ 3d^2$	[Ar] + + +
23	V	[Ar] $4s^2 3d^3$	[Ar] + + +
24	*Cr	[Ar] $4s^1 3d^5$	[Ar] + + + + - +
25	Mn	$[\mathbf{Ar}] \ 4s^2 \ 3d^5$	[Ar] + + + + +
26	Fe	[Ar] $4s^2 3d^6$	[Ar]
27	Co	[Ar] $4s^2 3d^7$	[Ar] 🛟 🛧 🛧 🛧 🛧 — — —
28	Ni	[Ar] $4s^2 3d^8$	[Ar] 1 + 1 + 1 + 1 +
29	*Cu	[Ar] $4s^1 3d^{10}$	
30	Zn	[Ar] $4s^2 3d^{10}$	
31	Ga	$[Ar] 4s^2 3d^{10} 4p^1$	
32	Ge	$[Ar] 4s^2 3d^{10} 4p^2$	
33	As	$[Ar] 4s^2 3d^{10} 4p^3$	
34	Se	[Ar] $4s^2 3d^{10} 4p^4$	
35	Br	[Ar] $4s^2 3d^{10} 4p^5$	
36	Kr	[Ar] $4s^2 3d^{10} 4p^6$	

*From Hund's Rule, Cr and Cu can achieved lowest energy if the $4s^2 e^-$ was moved to the $3d^5$ or $3d^{10}$.



Order of appearance for Subshell

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Some Exceptions in Electron Configurations



((Mair	n Gro	ups)												(M	lain C	iroup	s)	18
	s bl	ock															p blo	ock		8A
	1	2									- a [1			13	14	15	16	17	2
	IA	2A					Tra	nsitio	on Me	etals	15				3A	4A	5A	6A	7A	
2s	3	4						d b	lock					2p	5	6	7	8	9	10
	11	12	1	3	4	5	6	7	8	9	10	11	12	-	13	14	15	16	17	18
38				3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3p						
4s	19	20	3d	21	22	23	24	25	26	27	28	29	30	4p	31	32	33	34	35	36
58	37	38	4d	39	40	41	42	43	44	45	46	47	48	5p	49	50	51	52	53	54
6s	55	56	5d	71	72	73	74	75	76	77	78	79	80	6p	81	82	83	84	85	86
7s	87	88	6d	103	104	105	106	107	108	109	110	111	112	7p	113	114	115	116	117	118



Series 4f	57	58	59	60	61	62	63	64	65	66	67	68	69	70
Actinium 5f Series	89	90	91	92	93	94	95	96	97	98	99	100	101	102



7.12: Periodic Trends in Atomic Properties

There are many different trends regarding the physical and chemical properties of the elements in the Periodic Table. However, we will limit to three atomic properties. They are ionization energy, electron affinity, and atomic size.

Shielding Effect: - the outer electrons are pushed away because of the repulsion between them and the core electrons. The net result is that the protons in the nucleus cannot hold on to these outer electrons as tightly as they would for the core electrons.

atom



<u>Effective Nuclear Charge</u> (Z_{eff}): - the net nuclear charge actually experienced by an electron (the difference between the number of protons, Z, and the number of "shielded" core electrons).
 - the higher it is for Z_{eff}, the less shielding effect the outer electrons will experience.

$Z_{eff} = Z -$ "Shield" Core Electrons

Example 1: Calculate the effective nuclear charge of Na and Ar (first and last elements of period 3).

Sodium (Na):
$$Z = 11$$
 protons"Shield" Core $e^- = 10$ (e^- in the first two shells) $Z_{eff} = 11 - 10$ $Z_{eff} = 1$ for NaArgon (Ar): $Z = 18$ protons"Shield" Core $e^- = 10$ (e^- in the first two shells) $Z_{eff} = 18 - 10$ $Z_{eff} = 8$ for Ar(Ar has experience LESS shielding effect than Na)

Ionization Energy: - the energy needed to completely remove an electron from a gaseous atom or gaseous ion (plasma).

First Ionization Energy: - the ionization energy required to remove the highest-energy electron from an

<u>Second Ionization Energy</u>: - the ionization energy required to remove the second highest-energy electron from the ion.

 $X^{+}_{(g)} \rightarrow X^{2^{+}}_{(g)} + e^{-}$ $Na^{+}_{(g)} \rightarrow Na^{2^{+}}_{(g)} + e^{-}$ $I_2 = 4560 \text{ kJ/mol}$

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Elements	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	495	4560					
Mg	735	1445	7730		Core E	lectrons	
Al	580	1815	2740	11600	_		
Si	780	1575	3220	4350	16100		
Р	1060	1890	2905	4950	6270	21200	
S	1005	2260	3375	4565	6950	8490	2700
Cl	1255	2295	3850	5160	6560	9360	1100
Ar	1527	2665	3945	5770	7230	8780	1200

Successive Ionization Energies (kJ/mol) for Elements in Row 3 of the Periodic Table

Successive Ionization Energies INCREASES within each element. $(I_1 < I_2 < I_3 < ...)$

Several Notes on Trends in Ionization Energies

- 1. There is an <u>Increase in Successive Ionization Energies</u> because each successive electron has to jump from a lower level. Besides, these successive electrons are bind more tightly with the nucleus because they are closer to the protons.
- 2. <u>Ionization Energies Decrease Down a Group</u>. This is due to the fact as the atom has more orbitals, it is increasing in size. It is easier (takes less energy) to take away a valence electron because the protons are having a more difficult time to "hold on" to the electron.
- **3.** In general, <u>Ionization Energies Increase as one move from Left to the Right of a Period</u>. This is because the increases in protons in the same row increase the effective nuclear charge (the protons in the nucleus have more pull on the outer electrons, decreasing shielding), thus requiring more energy to ionize them.
- 4. The notable exceptions to the above statement is between Mg and Al along with P and S. In the case between magnesium and aluminum, the I_1 decreases because of the change in subshells ([Ne] $3s^2$ and [Ne] $3s^2 3p^1$). It is easier to remove a $3p^1$ electron than an electron in $3s^2$. Between P and S, the electron configuration changes between [Ne] $3s^2 3p_x^{-1} 3p_y^{-1} 3p_z^{-1}$ to [Ne] $3s^2 3p_x^{-2} 3p_y^{-1} 3p_z^{-1}$. Again, it is easier to remove an electron from a $3p_x^2$ orbital because of Hund's Rule (the lowest energy state is achieved when all electrons in the subshell is unpaired).



Electron Affinity: - the change in energy associates with an addition of an electron to a gaseous atom. - the larger negative electron affinity, the more stable the anion formed.

$$X_{(g)} + e^- \rightarrow X^-_{(g)}$$
Cl_(g) + $e^- \rightarrow Cl^-_{(g)}$ $\Delta EA = -348.7 \text{ kJ/mol}$ (348.7 kJ/mol is released)

Several Notes on Trends in Electron Affinities

- In general, <u>Electron Affinity DECRESES Down a Group (less energy is released)</u>. This is due to the fact there are more orbitals as the number of row increases. Since the protons in the nucleus cannot attract another electron as effectively due to the increase distance involved, less energy is released. <u>The trend holds except for row 2. The reason is because of the small size of the 2p orbitals. Electron repulsion cause smaller values of electron affinities than expected for row 2.</u>
- 2. In most cases, <u>Electron affinity INCRESASES (becomes more negative) across the Period from</u> <u>Left to Right up to the Halogen group (more energy is released)</u>. Metals have EA > 0 because they like to form cations (low ionization energy). Non-metals have EA < 0 because they like to form anions in order to form a stable octet.
- 3. Exceptions can be found in the 2A and 5A Groups. With the 2A Alkaline Earth Group, it is more difficult to add an electron into the *s* orbital such that it will be filled to $ns^2 np^1$. This is because the 2A Group already has an electron configuration of ns^2 (subshell is already filled). Therefore, they have a more positive (less negative) electron affinity. In the case of the 5A Group, the atoms find themselves difficult to add another electron because this will mean a np^4 configuration, which contains a paired electron from three unpaired electrons in np^3 . Again, Hund's Rule frowns on such arrangement because it is not of the lowest energy state. Thus, Group 5A tends to have a more positive (less negative) electron affinity.



Atomic Radius: - the size of an atom as measured by the distances between atoms in chemical compound.



Several Notes on Trends in Atomic Radii

- 1. In general, <u>Atomic Radii decrease as one move to the right of a period</u>. This is because the increases in protons in the same row increase the effective nuclear charge (the protons in the nucleus have more pull on the outer electrons, decreasing shielding), thus drawing these outer electrons closer to the nucleus, decreasing in sizes as the result.
- 2. <u>Atomic Radii INCRESES Down a Group</u>. This is due to the fact there are more orbitals as the number of row increases. The outer electrons are, of course, further away from the nucleus



Relative Atomic Sizes of the Representative Elements

Sizes of atoms tend to decrease across a period

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