VC210

Final Review

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December 12, 2018

- Fundamentals
- 2 The Quantum World
- 3 Atoms
- 4 Chemical Bonds
- Molecular Theories



Units

- Common units: Pound, Inch, Minute...
- SI Units: Kilogram (kg), Second (s), Kelvin (K)
- SI Prefixes:
 - mega-(M): 10^6
 - kilo-(k): 10^3
 - milli-(m): 10^{-3}
 - micro- (μ) : 10^{-6}
 - nano-(n): 10^{-9}

Significant Figures

 Addition and Subtraction: Round off the result to the leftmost decimal place.

$$40.123 + 20.34 = 60.46$$

 Multiplication and Division: Round off the result to the smallest number of significant figures.

$$1.23 \times 2.0 = 2.5$$

• Logarithms: retain in the mantissa the same number of SF as there are in the number whose logarithm you are taking.

$$\log 12.8 = 1.107$$

Exponents: The number of SF is the same as in the mantissa.

$$10^{1.23} = 17$$

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Nuclear Model of the Atom

- $e = 1.602 \times 10^{-19} C$
- $m_e = 9.109 \times 10^{-31} kg$
- Rutherford's model of atom: All the positive charge and almost all the mass is concentrated in the tiny nucleus, and the negatively charged electrons surround the nucleus.

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Electromagnetic Radiation

- Speed of light: $c = 3 \times 10^8 m \cdot s^{-1}$
- $1Hz = 1s^{-1}$
- $\lambda \times v = c$



Some Important Formula

•
$$v = R(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

- Rydberg constant: $R = 3.29 \times 10^{15} Hz$
- Wave-Particle Duality of Matter: $E=hv=rac{hc}{\lambda}$
- de Broglie Relation: E = pc(p is momentum)
- A Particle in the Box: $E_n = \frac{n^2 h^2}{8mL^2}$

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Quantum Numbers

- Principal quantum number n(shell)
- ullet Orbital angular momentum quantum number $l \in [0,n-1]$ (subshell)
 - l = 0(s), l = 1(p), l = 2(d)...
- Magnetic quantum number $m_l \in [-l, l]$ (orbitals)
- ullet Spin magnetic quantum number $\mathit{m_s} \in \{rac{1}{2}, -rac{1}{2}\}$



Atomic Orbitals

- Nodes: n-1
- Radial(spherical) nodes: n-l-1
- Angular(planer) nodes: /



The Building-Up Principle

- Pauli Exclusive Principle: no two electrons in one atom have the same four quantum number.
- Lowest Energy Principle: electrons tend to enter orbitals with lower energy first.
 - Energy ranking: 1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < ...
- Hund's Rule: For degenerate orbitals, the lowest energy is attained when the number of electrons having same spin is maximized.
- Hund's exception: For same subshell, when electrons are full or half-full or empty, it is most stable.(Cu)



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Periodicity

- Atomic Radius:
 - Same row: radius decreases from left to right.
 - Same column: radius increase from up to down.
- Ionization Energy: minimum energy needed to remove an electron from an neutral gas phase atom. Mostly increases from the lower left corner to upper right corner.
- Electron Affinity: Energy released when an electron is added to gas phase atom. Mostly increases from the lower left corner to upper right corner.

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Lewis Symbols

- Three bond types: metal bond, ionic bond, covalent bond.
- For Lewis symbols: a single dot represents a valence electron, double dots represent a lone pair of electrons, one line represents a bond (pair electrons).

H· He:
$$:\dot{N}\cdot \cdot \dot{G}\cdot :\dot{G}\cdot K\cdot Mg$$
: $:\dot{F}\cdot + \dot{F}: \longrightarrow (:\dot{F}:)\dot{F}:)$, or $:\dot{F}-\dot{F}:$

Draw Linkage for Polyatomic Molecules

SOLVE

Step 1 Count the valence electrons and adjust the number for charges on ions.

Count the electron pairs.

Step 2 Arrange the atoms.

Step 3 Place one electron pair between each pair of bonded atoms.

Step 4 Count electron pairs not yet located.

Complete the octets with lone pairs. If there are not enough electrons to give each atom an octet or duplet with single bonds, use multiple bonds.

Step 5 Represent the bonds by lines and indicate charges.

(a) H ₂ O	(b) H ₂ CO	(c) CIO ₂
1+1+6=8	1+1+4+6=12	7 + 6 + 6 + 1 = 20
4	6	10
	Н	
н о н	C O	O CI O
	Н	
	Н	
н:о:н		o: cl: o
н.о.н	c : o	0.0.0
	Н	
:: (2)	::: (3)	::::::::(8)
	Н	
н: ё: н	c :: Ö	:0 : 0 : 0:
н. й. н	Н	.g . g . g.
	H	
	c—;;	7-
н—о—н	c=ö	:o-ci-o:
	H	

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Resonance

- Keep relative position of atoms.
- Only change electron configuration.
- All atoms in resonance should be coplanar.
- Number of paired and unpaired electrons keep unchanged.
- Bond Order:

Number of bonds at the same positions in all its resonance structures number of resonance structures

$$\vdots \ddot{0} : \ddot{0}$$

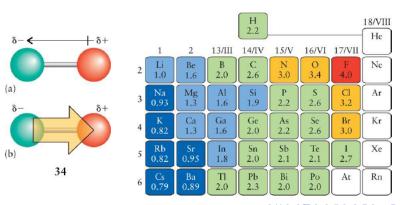
Formal Charge

- Formal Charge = $V (L + \frac{1}{2}B)$
 - V: number of valence electrons
 - L: number of lone-pair electrons
 - B: number of bonding electrons
- Formal charges closest to zero represents the lowest energy arrangement of the atoms.

$$-1$$
 +1 0 -1 +2 -1
 $N = N = O$ $N = O = N$

Electric Dipole Moment

- Elements with higher electronegativity values are considered as negative poles. With larger differences in electronegativity, the dipole moment is larger.
- There are two different drawings.



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To find geometry:

- Draw the lewis structure.
- Find AX_nE_m .
 - A: central atom
 - X: number of bonds
 - E: number of lone pairs
- Search the table and find.

Number of Electron Domains	Electron- Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
2	Linear	2	0	Linear	ö=c=ö
3	Trigonal planar	3	0	Trigonal planar	#:
		2	1	Bent	

Number of Electron Domains	Electron- Domain Geometry	Bonding Domains	Nonbending Domains	Molecular Geometry	Example
4	Tetrahedral	4	0	Tetrahedral	Hang H
		3	1		H ^{wr.} N
		2	2	Trigonal pyramidal	H ^{w.} Ö.

Number of Electron Domains	Electron- Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
5	of the second	5	0	*	PCl ₅
	Trigonal bipyramidal			Trigonal bipyramidal	
		4	1	Seesaw	SF_4
		3	2	T-shaped	CIF ₃
		2	3	Linear	XeF_2

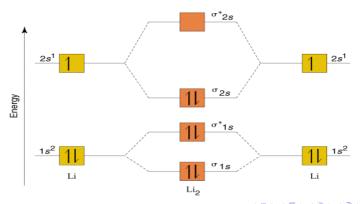
Number of Electron Domains	Electron- Domain Geometry	Bonding Domains	Nonbonding Domains	Molecular Geometry	Example
6	Octahedral	6	0	Octahedral	SF ₆
		5	í	Squaro pyramidal	ВтF5
		4	2		XeF ₄

Valence Bond Theory

- σ -bond and π -bond: single bond is a σ -bond, double bond is a σ -bond plus a π -bond, triple bond is a σ -bond plus two π -bonds.
- Hybridization: k = m + n, m is the number of lone pairs of central atom, n is the number of atoms connected to central atom.
 - sp: k = 2
 - $sp^2 : k = 3$
 - $sp^3 : k = 4$
 - $sp^3d : k = 5$
 - $sp^3d^2: k = 6$

Molecular Orbital Theory

- The number of MOs equals the number of AOs.
- The MO can be classified as bonding, nonbonding and antibonding.
- $E(\sigma_{1s}) < E(\sigma_{1s}^*)$
- The number of electrons is unchanged.



Molecular Orbital Theory

- Be sure to remember the order of the following MO diagram.
- More electronegative element has lower energy.
- Bond Order: $\frac{1}{2}(N_{bonding} N_{antibonding})$
- Paramagnetic: has unpaired electrons.
- Diamagnetic: all electrons are paired.

Large 2s-2p interaction			Small 2s-2p interaction				
	B ₂	C ₂	N ₂		O ₂	F ₂	Ne ₂
σ_{2p}^*				σ_{2p}^{\star}			11
π_{2y}^*				π_{2p}^*	1 1	11 11	11 11
σ_{2p}			11	π_{2p}	11 11	11 11	11 11
π_{2p}	1 1	11 11	11 11	σ_{2p}	11	11	11
σ_{2s}^*	11	11	11	σ_{2s}^{\star}	11	11	11
σ_{2s}	11	11	11	σ ₂ ,	11	11	11

Good Luck!