(1) **Today**

Attendance

Review Syllabus

Sections 1.1 – 1.3 atomic structure electrons, valence vs core electrons

Reviewing Periodic Trends

Section 1.4 Introduction to Chemical Bonding Theories octet rule etc

(3) Second Class from Today

Sections 1.5-1.10 Valence Bond Theory

Skipping Section 1.11 for now An introduction to Molecular Orbital Theory

Sections 1.12 Drawing Chemical Structures

Next Class (2)

Section 1.4 Introduction to Chemical Bonding Theories octet rule etc

> Sections 1.5-1.10 Valence Bond Theory

Third Class from Today (4)

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

> Sections 2.4 – 2.6 Resonance/Electron Delocalization

Atoms, Elements, Molecules, and Substituents or Groups

Ch indecule

A diversion into the language of chemistry...

) گ

"In chemistry, an element is a pure substance consisting only of atoms that all have the same numbers of protons in their atomic nuclei."¹



¹ <u>https://en.wikipedia.org/wiki/Chemical_element</u> accessed September 3, 2021

Remember the structure of an atom

And Where Are the Electrons Again?

Bohr



First person to model the atom with quantized energy levels starting from basic particle physics; e.g.,

 $E = KE + PE \quad or \quad E = 1/2 \ mv^2 + Ze^2/r$ centripetal force = mv²/r force of attraction between charged particles = Ze²/r²

Only worked for atoms with one electron.

Also it is physically impossible for electrons to orbit a nucleus like the Moon orbits the Earth.... The electrons would radiate energy and crash into the nucleus.

And Where Are the Electrons Again?

Sections 1.1 – 1.3



Image derived from https://en.wikipedia.org/wiki/Atom#/media/File:Helium_atom_QM.svg

Wave/Quantum Mechanical Model



1 Å = 100 pm

Bohr had 1 quantum number.

05-1

the electron is in the n = 1 or 2 or 3 or 4... shell

Quantum Mechanics requires four quantum numbers to describe an electron: n, l, m_l , and m_s .

n is the principal energy level l describes the shape of the orbital \mathbf{m}_l describes the orientation of the orbital and \mathbf{m}_s indicated the spin of the electron.

Further, as \vec{n} gets larger more orbital shapes become available and as more shapes become available more orientations become possible



And Where Are the Electrons Again?

Sections 1.1 – 1.3





Remember how electrons are distributed, electron configuration Remember the importance of valence electrons/the valence shell

Example Electron configurations



Sections 1.1 – 1.3

Use the periodic table to identify metals and non-metals

Use the periodic table to remember trends in size

Use the periodic table to remember trends in electronegativity

Use trends in size, electron configuration, and nuclear charge to explain electronegativity trend

Use the periodic table to predict likely bond formation

Introduce Valence Bond Theory (hybridization)



The Periodic Table Is Your Friend and Basic Bonding Theory

Review



Predict the number of electrons or bonds needed for an element to form a stable compound room for 1 e nears room to form 1 covalent bond

19

The Periodic Table Is Your Friend: Metals tend to gain and nonmetals tend to lose electrons

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Fe	C	CaK	NCa	Cu	۱	Ga	G	e A	s	Se	Br	Kr	C	u	Zn	Ga	Ge	As	Se	Br	Kr
44	45	537 4	638 4	73	4	49	50	51	5	52	53	54	47		48	49	50	51	52	53	54
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76	7	755 7	856 7	95	7	81	82	83	8	34	85	86	79	79 80		81	82	83	84	85	86
Os		lrCs	PBa	Aψ	J	TI	P	o E	Bi	Po	At	Rn	A	u	Hg	ΤI	Pb	Bi	Po	At	Rn
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Review

1s² 2s² 2p⁵

F

Why

Review

1]																2
Н																	He
3	4						5	6	7	8	9	10					
Li	Be						В	С	Ν	0	F	Ne					
11	12						13	14	15	16	17	18					
Na	Mg						AI	Si	Р	S	CI	Ar					
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Со	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	I	Xe
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ва	La	Hf	Та	W	Re	Os	lr	Pt	Au	Hg	TI	Pb	Bi	Ро	At	Rn
87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	FI	Мс	Lv	Ts	Og

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Ра	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Remember periodic trends

Ionic Interactions, Polar Bonds, and Nonpolar Bonds

NaCl Na⁺ and Cl⁻

HF H—F

H-H

 H_2

¹https://en.wikipedia.org/wiki/Sodium_chloride#/media/File:NaCl_bonds.svg

Review (and Section 2.1)



Electronegativity

Review



 $\Delta H_{BDE} = 436 \text{ kJ/mol}^{1}$

 $\Delta H_{BDE} = 155 \text{ kJ/mol}^{1}$

assuming BDE is average of H_2 and F_2 BDE predict $\Delta H_{BDE} = 296$ kJ/mol ?

1																								2
Н																								He
3	4																5	6		7		8	9	10
Li	Be																В	0	2	N		0	F	Ne
11	12																13	14		15		16	17	18
Na	Mg	9															Al	S	Si	F)	S	CI	Ar
19	20	21		22	23	24		25	26	27		28		29	30		31	32		33		34	35	36
K	Ca	a S	SC	Ti	\	/ C	r	Mn	F	e C	0	Ν	i	Cu	Z	n	Ga	G	ie	A	s	Se	Br	Kr
37	38	39		40	41	41 42		43	44	45		46		47	48		49	50	50			52	53	54
Rb	Si	· `	Y	Zr Nb Mo		lo	Тс	R	u R	lh	Po	b	Ag	C	d	In	S	Sn		b	Те		Xe	
55	56	57		72	73	74	4 75		76	77		78	79		80		81	82	82			84	85	86
Cs	Ba	a L	a	Hf	T	a V	V	Re	0	s Ir		Pt		Au Hạ		g	TI	P	Pb		i	Ро	At	Rn
87	88	89		104	10	5 10	6	107	108	3 109		110	110 111		112	112		3 114		115	5	116	117	118
Fr	Ra	Ra Ac		Rf	D	b S	g	Bh	H	s N	/It	Ds	S	Rg	C	n	Nh	F	-1	M	с	Lv	Ts	Og
	ſ								60		•••	7	0	74										
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	·		Th Pa U		U	Np	P	u A	١m	Cm	E	3k	С)f	Es	F	m	Md	No		Lr			

Remember periodic trends

Review

High energy electrons are reactive

low energy electrons are less reactive

(4) **Today**

Section 1.4 Introduction to Chemical Bonding Theories octet rule etc

Sections 1.5-1.10 Valence Bond Theory

(6) Second Class from Today

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

Sections 2.4 – 2.6 Resonance/Electron Delocalization

Bring Modeling Kits to Class

Next Class (5)

Sections 1.5-1.10 Valence Bond Theory

Sections 1.12 Drawing Chemical Structures

Third Class from Today(7)

Sections 2.7 – 2.11 Acids and Bases An Introduction to Valence Bond Theory

Section 1.4





Bring Modeling Kits to Lab this Week

Wait, what can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

Why is there free rotation around C to C single bonds but not C to C double bonds?

Which bond is stronger?

Explain observations and make predictions based on Valence Bond Theory

An Introduction to Valence Bond Theory

Sections 1.4









Just a Reminder that what I just said about orbitals being the "wrong" shape isn't Section 1.11+ a problem in MO theory



one 2s orbital and three 2p orbitals from one C atom

four 1s orbitals from four H atoms





https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid.html Identify atoms that use sp³ hybrid orbitals to form bonds and hold lone-pair electrons



https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid.html Identify atoms that use sp³ hybrid orbitals to form bonds and hold lone-pair electrons



Identify atoms that use sp³ hybrid orbitals to form bonds and hold lone-pair electrons

(5) **Today**

Section 1.4 Introduction to Chemical Bonding Theories octet rule etc

Sections 1.5-1.10 Valence Bond Theory

Sections 1.12 Drawing Chemical Structures

(7) Second Class from Today

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

Sections 2.4 – 2.6 Resonance/Electron Delocalization

Bring Modeling Kits to Class

Next Class (6)

Sections 1.12 Drawing Chemical Structures

Third Class from Today(8)

Sections 2.7 – 2.11 Acids and Bases hybrid orbitals are used to form σ bonds and to hold lone-pair electrons

in the valence bond model, single bonds are always σ bonds

double and triple bonds are formed from σ bonds plus π bonds

of σ bonds + pairs of lone-pair electrons = # of hybrid orbitals needed

or

number of directions electrons must be pointed in = # of hybrid orbitals needed

count out the # of atomic orbitals need to make the hybrid orbitals starting with the 2s orbital (or 3s if appropriate)

name the hybrid orbitals spⁿ where n is the number of p orbitals used



https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid2.html Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons



https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid2.html

Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons

 CH_3^+

 CH_3^-

 ${CH_3}^{\bullet}$

Determine the hybridization of unusual molecular fragments

(6) **Today**

Sections 1.5-1.10 Valence Bond Theory

Sections 1.12 Drawing Chemical Structures

Next Class (7)

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

> Sections 2.4 – 2.6 Resonance/Electron Delocalization

(8) Second Class from Today

Sections 2.4 – 2.6 Resonance/Electron Delocalization

Sections 2.7 – 2.11 Acids and Bases

Third Class from Today(9)

Sections 2.7 – 2.11 Acids and Bases What can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

Why is there free rotation around C to C single bonds but not C to C double bonds?

Which bond is stronger?

Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

What can we use Valance Bond Theory for?

Why is there free rotation around C to C single bonds but not C to C double bonds?



Explain observations and make predictions based on the hybridization of an atom
What can we use Valance Bond Theory for?

Which bond is strongest? 370 kJ/mol², 355±8 kJ/mol³

426 kJ/mol¹

490 kJ/mol⁴







² Organic Chemistry, 10th ed. McMurry.

³ Chem. Rev. **66**, 465 (1966).

⁴ J.Chem.Ed. **42**, 502 (1965)

Practice







Sections 1.12 Drawing Chemical Structures

Next Class (8)

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

> Sections 2.4 – 2.6 Resonance/Electron Delocalization

(9) Second Class from Today

Sections 2.4 – 2.6 Resonance/Electron Delocalization

Sections 2.7 – 2.11 Acids and Bases

Third Class from Today(10)

Sections 2.7 – 2.11 Acids and Bases Lewis & Kekulé Structures

Section 1.12

H H H H:C:O:C:C:H H H H

Chemists use different drawings to place emphasis on different aspects of a molecule.

Representations are used to solve typographical issues.

Molecular Formulas as Compared to Condensed Structures/Structural Section 1.12 Formulas

In organic, molecular formulas are written C_xH_y (and other elements listed alphabetically)

 C_3H_8O

Molecular Formulas as Compared to Condensed Structures/Structural Section 1.12 Formulas

In organic, condensed structures typically start with a C, and everything immediately to the right of the C is connected to that first C. When the the first C is finally connected to the second C, now that atoms right of the second C are connected to second C. In acyclic unbranched molecules atoms to the right of the second C are not connected to the first C.

 C_3H_8O

CH₃CH₂OCH₃

CH₃CH₂CH₂OH

CH₃CHOHCH₃

In organic, condensed structures typically start with a C, and everything immediately to the right of the C is connected to that first C. When the first C is finally connected to the second C now that atoms right of the second C are connected to second C. In acyclic unbranched molecules, atoms to the right of the second C are not connected to the first C.

CH₂CHCH₃

Because bonds are not drawn, condensed structures require the reader to bring some chemical knowledge to their interpretation.

Section 1.12



 $CH_3CH(OH)CH_2CH_3$ $CH_3(CH_2)_3CH_3$ $CH_3CH_2CH(CH_3)_2$

Parentheses () in structures are typically used to set off side chains, to indicate a repeating unit, or to indicate multiple groups of the same structure.

Condensed Structures/Structural Formulas

Section 1.12

Often, chemists omit parentheses when they are not absolutely necessary,

СΠ3	(UI	٦ ₂)	'3'	пз

CH₃CHOHCH₃ CH₃CH(OH)CH₃

 $CH_3COCH_2CH_3$ $CH_3C(O)CH_2CH_3$

and sometimes chemists do things for aesthetic reasons.

 $C(CH_3)_3OH$ $CH_3C(CH_3)_2OH$ $(CH_3)_3COH$

Section 1.12

 $CH_3CHOHCH_2CH_3$

 $CH_3C(O)CH(CH_3)_2$

CH₃CHO

When a bond ends and the atom isn't labeled it is assumed to be C.

When there aren't enough bonds drawn to a C atom, the "missing" bonds are C atom to H atom bonds.

All other atoms are labeled.

Heptane CH₃CH₂CH₂CH₂CH₂CH₂CH₃

2-heptanol CH₃CHOH(CH₂)₄CH₃

Different structures serve different purposes, but they represent the same things

Converting Between Structure Types





$CH_{3}CH(OH)CH_{2}CH(CH_{3})CH_{2}CH_{3}$

(8) **Today**

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

Section 2.1: Problems 2-1 – 2-4 Section 2.2: Problems 2-5, 2-6, 2-28 – 2-30, 2-32, 2-53, 2-59, 2-63 Section 2.3: Problems 2-7, 2-8, 2-35, 2-36

(10) Second Class from Today

Sections 2.7 – 2.11 Acids and Bases

2.7 Acids and Bases: The Brønsted–Lowry Definition
Problem 2-11
2-8 Acid and Base Strength
Problem 2-12, 2-13
2.9 Predicting Acid–Base Reactions from pKa Values
Problem 2-14 – 2-16
2.10 Organic Acids and Organic Bases
2.11 Acids and Bases: The Lewis Definition
Problem 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acid-base concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

Next Class (9)

Sections 2.3 – 2.7 Formal Charges, Resonance/Electron Delocalization

Sections 2.4 – 2.6: Problem 2-9, 2-10, 2-20, 2-21, 2-23, 2-26, 2-37, 2-38, 2-56, 2-57, 2-61, Challenging Problems 2-33, 2-34, 2-39

Third Class from Today (11)

Sections 2.7 – 2.11 Acids and Bases

Section 2-12 Non-Covalent Interactions Between Molecules

2.12 Noncovalent Interactions between Molecules Problem 2-19, 2-65 "As a rough guide, bonds between atoms whose electronegativities differ by less than 0.5 are [considered] nonpolar covalent, bonds between atoms whose electronegativities differ by 0.5 to 2 are polar covalent, and bonds between atoms whose electronegativities differ by more than 2 are largely ionic."⁵





Today's Office Hours are canceled. I have a meeting in Fitchburg that I have to get to.

³ Organic Onemistry, 10⁴¹ ed., iviciviurray, OpenStax (2023) https://openstax.org/details/books/organic-cnemistry







Draw Lewis Structure

Draw VSEPR Structure

Draw Dipole arrows on polar bonds

If (+) and (-) are on opposite sides (front and back, left and right, top and bottom, upper left and lower right) then the molecule is polar otherwise it isn't.

 $CH_2CI_2 \\$

Draw Lewis Structure

Draw VSEPR Structure

Draw Dipole arrows on polar bonds

If (+) and (-) are on opposite sides (front and back, left and right, top and bottom, upper left and lower right) then the molecule is polar otherwise it isn't.



Draw Lewis Structure

Draw VSEPR Structure

Draw Dipole arrows on polar bonds

If (+) and (-) are on opposite sides (front and back, left and right, top and bottom, upper left and lower right) then the molecule is polar otherwise it isn't.



(9) **Today**

Sections 2.1 - 2.4 Polar Covalent Bonds, Formal Charges, Resonance/Electron Delocalization

Section 2.1: Problems 2-1 – 2-4 Section 2.2: Problems 2-5, 2-6, 2-28 – 2-30, 2-32, 2-53, 2-59, 2-63 Section 2.3: Problems 2-7, 2-8, 2-35, 2-36

(11) Second Class from Today

Sections 2.7 – 2.11 Acids and Bases

Section 2.7: Problem 2-11 Section 2.8: Problems: 2-12, 2-13 Section 2.9: Problems 2-14 – 2-16 Section 2.10 - 2:11: 2.11 Problems: 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acid-base concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

Next Class (10)

Sections 2.3 – 2.7 Formal Charges, Resonance/Electron Delocalization

Sections 2.4 – 2.6: Problem 2-9, 2-10, 2-20, 2-21, 2-23, 2-26, 2-37, 2-38, 2-56, 2-57, 2-61, Challenging Problems 2-33, 2-34, 2-39

Third Class from Today (12)

Sections 2.7 – 2.11 Acids and Bases

Section 2-12 Non-Covalent Interactions Between Molecules

2.12 Problems: 2-19, 2-65

Formal Charge	# valence e⁻'s in		# of lone pair		1/2 of the e-'s	
of an atom	the neutral atom	-	electrons	+	in the bonds	



Formal Charge		# valence e-'s in	1	# of lone pair		1/2 of the e-'s	٦		
of an atom	=	the neutral atom	-		electrons	+	in the bonds)

 $CH_{3}OH$

Section 2.3





Formal Charge		# valence e-'s in		1	# of lone pair		1/2 of the e [_] 's	\
of an atom	=	the neutral atom	-		electrons	+	in the bonds)



Also a way to move charge around a molecule...

Which one is correct?



Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.





Resonance: Where else do we see extended π systems/electron delocalization



Vitamin C

Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



Resonance: The resonance hybrid resembles...

The more stable the resonance contributor is, the more it contributes to the resonance hybrid

- 1. Incomplete octets
- 2. "Wrong" charges
 - negative charge is not on the most electronegative element
 - a positive charge on an electronegative element
- 3. charge separation



Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



Resonance: Empty orbitals

Whenever 3 or more p orbitals are in a row, experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



(12) Second Class from Today

Sections 2.7 – 2.11 Acids and Bases

Section 2-12 Non-Covalent Interactions Between Molecules

2.12 Problems: 2-19, 2-65

(10) **Today**

Sections 2.3 – 2.7 Formal Charges, Resonance/Electron Delocalization

Sections 2.4 – 2.6: Problem 2-9, 2-10, 2-20, 2-21, 2-23, 2-26, 2-37, 2-38, 2-56, 2-57, 2-61, Challenging Problems 2-33, 2-34, 2-39

Next Class (11)

Sections 2.7 – 2.11 Acids and Bases

Section 2.7: Problem 2-11 Section 2.8: Problems: 2-12, 2-13 Section 2.9: Problems 2-14 – 2-16 Section 2.10 - 2:11: 2.11 Problems: 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acid-base concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

Third Class from Today (13)

Section 3.1 Functional Groups

Section 3.2 Alkanes and Isomers

> Section 3.3 Alkyl Groups

Section 3.4 Nomenclature

Drawing Resonance Contributors

Rules for drawing Resonance Contributors

- 1. atoms don't move, only electrons
- 2. don't move σ bonds, only π bonds, lone pair e-'s, or unpaired e-'s (radicals)
- 3. the total number of electrons must stay the same, **don't change the net charge**
- 4. p orbitals must be able to line up parallel to each other



Drawing Resonance Contributors

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Drawing Resonance Contributors

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- 3. the total number of electrons must stay the same, **don't change the net charge**
- 4. p orbitals must be able to line up parallel to each other



Acids and Bases and Language

In aqueous solutions, the solution is considered **acidic** if the concentration of **H**⁺ is **greater than** the concentration of **OH**⁻. At 25 °C, this occurs when the pH is less than 7.

In every day language, we might say that the solution is an acid. More precisely, there is a molecule **in the solution that acing as an acid and is causing the solution to be acidic**.

We will call molecules or ions acids or bases based on how they react (or could react).

There are **many molecules** that can **act as a base** in some circumstances **or an acid** in other circumstances. Acids and Bases and Language

Molecules or compounds that are very likely to react as an acid are often called acids, but technically, the molecules are referred to as acids and bases based on how they react.

HNO₃, for example...

(11) **Today**

Sections 2.7 – 2.11: Acids and Bases

Section 2-12: Non-Covalent Interactions Between Molecules

Section 2.7: Problem 2-11 Section 2.8: Problems: 2-12, 2-13 Section 2.9: Problems 2-14 – 2-16 Section 2.10 - 2:11: 2.11 Problems: 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acid-base concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

(13) Second Class from Today

Section 3.1 Functional Groups

Section 3.2 Alkanes and Isomers

Section 3.3 Alkyl Groups

Section 3.4 Nomenclature Section 2-12 Non-Covalent Interactions Between Molecules

2.12 Problems: 2-19, 2-65

Third Class from Today (14)

Section 3.1 Functional Groups

Section 3.2 Alkanes and Isomers

> Section 3.3 Alkyl Groups

Section 3.4 Nomenclature

Next Class (12)

A Brønsted-Lowry acid is a proton, H⁺, <u>DONOR</u>

A Brønsted-Lowry base is a proton, H⁺, <u>ACCEPTOR</u>.

Section 2.7











 $K_a \,and \, pK_a$

$HA(aq) \implies H^+(aq) + A^-(aq)$

$$pK_a = -log K_a$$

$$pH = pK_a + \log \frac{[A^-]}{[HA]} \qquad pH = pK_a + \log \frac{[A^-]}{[HA]}$$



pKa's CH₄, ~50 NH₃, ~36 H₂O, 15.6 HF, 3.18

pK_a - Which is the stronger acid?



(12) **Today**

Sections 2.7 – 2.11: Acids and Bases

Section 2-12: Non-Covalent Interactions Between Molecules

Section 2.7: Problem 2-11 Section 2.8: Problems: 2-12, 2-13 Section 2.9: Problems 2-14 – 2-16 Section 2.10 - 2:11: 2.11 Problems: 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acid-base concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

(14) Second Class from Today

Section 3.2: Alkanes and Isomers

Section 3.3: Alkyl Groups

Section 3.4: Nomenclature

Section 2-12: Non-Covalent Interactions Between Molecules

2.12 Problems: 2-19, 2-65

Section 3.1: Functional Groups

Section 3.2: Alkanes and Isomers

Third Class from Today (15) Test 1 on Chap 1 and 2

Next Class (13)

Section 2.6

The one that leaves the more/most stable base behind



Same Period More Positive Nucleus



pKa's CH₄, ~50 NH₃, ~36 H₂O, 15.6 HF, 3.18

Five ways to stabilize the electrons on the conjugate base

Section 2.6 - 2.9

Same Column Larger Valence Shell



Resonance



Inductive Effect



acetic, 4.76; formic, 3.75; chloroacetic, 2.87; dichloroacetic, 1.25

Greater s character



Practice: For each molecule, which proton is the most likely to be lost and for each pair, which is the stronger acid







.OH





(13) **Today**

Sections 2.11: Lewis Acids and Bases

Section 2-12: Non-Covalent Interactions Between Molecules

2.11 Problems: 2-17, 2-18, 2-24, 2-25, 2-40 (2-42 is a good question but theLewis acidbase concept is not strongly emphasized in our organic class), 2-43, 2-44, 2-46, 2-47, 2-48, 2-54, 2-55, 2-61, 2-64

Section 3.1: Functional Groups

Section 3.2: Alkanes and Isomers

(15) Second Class from Today

Test 1 on Chap 1 and 2

Next Class (14)

Section 3.2: Alkanes and Isomers

Section 3.3: Alkyl Groups

Section 3.4: Nomenclature

Third Class from Today (16)

Lewis Acids

Lewis Acids

intermolecular forces, van der Waals forces, or noncovalent interactions

London Dispersion Forces (LDF)

All molecules interact with other molecules using LDFs Interaction between spontaneous, random dipoles and induced dipoles Weak for molecules with few valence electrons and low surface area Strength increases with increasing valence electrons, surface area, and volume

Dipole-dipole interactions

Occurs between opposite ends of dipoles on polar molecules Presence of dipole dipole interactions can have a substantial affect on attraction between molecules

H Bond interactions

Occurs between H-bond donors and H-bond acceptors The strongest of these intermolecular forces (on an interaction by interaction basis) Important for water solubility and in biochemistry

intermolecular forces, van der Waals forces, or noncovalent interactions





40.2 °C





36.4 °C

117 °C

35.9 °C

intermolecular forces, van der Waals forces, or noncovalent interactions

dipole-dipole interactions





intermolecular forces, van der Waals forces, or noncovalent interactions

London dispersion forces (sometimes called dispersion forces)



intermolecular forces, van der Waals forces, or noncovalent interactions

Hydrogen bonds or H-bonds



intermolecular forces, van der Waals forces, or noncovalent interactions

A hydrogen bond requires an H-Bond donor and an H-bond acceptor



H-bond donor

any H atom that is covalently bonded to an N, O, or F atom

H-bond acceptor any N, O, or F atom





deoxycytidine monophosphate

deoxygaunosine monophosphate



deoxyadenosine monophosphate

deoxythymidine monophophate







60 g/L and 0.038 g/L

(14) **Today**

Finish Chap 2

Section 3.1: Functional Groups

Section 3.2: Alkanes and Isomers

(16) Second Class from Today

Section 3.2: Alkanes and Isomers

Section 3.3: Alkyl Groups

Section 3.4: Nomenclature

Next Class (15)

Test 1 on Chap 1 and 2 though section 2.10 (Monday's class)

Third Class from Today (17)

Section 3.4 Nomenclature

Section 3.5 - 3.7 Properties and Conformations of Alkanes

Chap 4 Cycloalkanes
Functional Groups

A **functional group** is a group of atoms within a molecule that has a characteristic chemical behavior.⁶





⁶ Organic Chemistry, 10th ed. McMurry. (2023) Openstax

Functional Groups: Alkanes and Alkenes and Alkynes

Section 3.1



branched, acyclic alkane

branched, acyclic alkenes

Functional Groups: Alkanes and Alkenes

Section 3.1



Formulas?





(15) **Today**

Section 3.1 Functional Groups

Section 3.2 Alkanes and Isomers

Section 3.3 Alkyl Groups

Section 3.4 Nomenclature

(17) Second Class from Today

Chap 4 Cycloalkanes

Next Class (16)

Section 3.4 Nomenclature

Section 3.5 - 3.7 Properties and Conformations of Alkanes

Chap 4 Cycloalkanes

Third Class from Today (18) Chap 4 Cycloalkanes













Organophosphates





Functional Groups: Carbonyl Compounds





Functional Groups: Carbonyl Compound with adjacent C's or H's

Section 3.1





Aldehydes



 $R_1 \text{ or } R_2 \neq H$

 R_1 or $R_2 = H$

Functional Groups: Carbonyl Compounds with Adjacent Polar Groups

Carboxylic Acids and Esters





 $R_1 = H \text{ or } R_1 \neq H$



Amides



Section 3.1



Functional Groups

Section 3.1

A list of some functional groups grouped to highlight which ones have similar reactivities



Nomenclature of Alkanes

Early names were based on the number of C atoms in the alkane, and the names came from a variety of places — and we're "stuck" with them for the first four

CH₃OH methanol the name is derived from a word coined by French chemists, Jean-Baptiste Dumas and Eugene Peligot, from "methy" (Greek for alcoholic liquid)" + hylē (Greek for "forest, wood, timber, material")⁷

CH₃CH₂OH "eth" to distinguish it from méthylène derived from French and German chemists "äthyl" in German⁸

CH₃CH₂CO₂H based on observation that it was the first (shortest chained) carboxylic acid that behaved like a fatty acid pro (from protos for first) + pion (from pion for fat) => propionic acid⁹

 $CH_3CH_2CH_2CO_2H$ isolated from butter => butyric acid¹⁰

⁷ https://en.wikipedia.org/wiki/Methanol#History

⁸ https://chemistry.stackexchange.com/questions/142839/why-is-ethane-in-methane, https://gallica.bnf.fr/ark:/12148/bpt6k6569005x/f15.item

⁹ https://en.wikipedia.org/wiki/Propionic_acid

¹⁰ https://en.wikipedia.org/wiki/Butyric_acid

Nomenclature of Alkanes: Original Scheme based names on number of C atoms present

methane	CH4
ethane	C_2H_6
propane	C ₃ H ₈
butane	C_4H_{10}
pentane	C ₅ H ₁₂
hexane	C ₆ H ₁₄
heptane	C7H16
octane	C ₈ H ₁₈
nonane	C ₉ H ₂₀
decane	C ₁₀ H ₂₂
undecane	C ₁₁ H ₂₄
dodecane	C ₁₂ H ₂₆

(16) **Today**

Section 3.1 Functional Groups

Section 3.2 Alkanes and Isomers

Section 3.3 Alkyl Groups

Section 3.4 Nomenclature

(18) Second Class from Today

Chap 4 Cycloalkanes

Next Class (17)

Section 3.4 Nomenclature

Section 3.5 - 3.7 Properties and Conformations of Alkanes

Chap 4 Cycloalkanes

Third Class from Today (19) Chap 4 Cycloalkanes

Nomenclature of Alkanes: Original Scheme based names on number of C atoms present but nonsystematic nomenclature becomes problematic quickly....

methane	CH ₄	1 isomer
ethane	C_2H_6	1 isomer
propane	C_3H_8	1 isomer
butane	C ₄ H ₁₀	2 isomers
pentane	C ₅ H ₁₂	3 isomers
hexane	C ₆ H ₁₄	5 isomers
heptane	C ₇ H ₁₆	
octane	C ₈ H ₁₈	
nonane	C ₉ H ₂₀	
decane	C ₁₀ H ₂₂	
undecane	C ₁₁ H ₂₄	
dodecane	$C_{12}H_{26}$	

But before getting into the systematic nomenclature of Substituted Alkanes: non-IUPAC names based on total number of C atoms present

iso-		R
isobutane	R = CH₃ (4 C's)	
isopentane	R = CH ₂ CH ₃ (5 C's)	
isohexane	R = CH ₂ CH ₂ CH ₃ (6 C's)	
neo-		R
neopentane	R = H (5 C's)	
neohexane	R = CH ₃ (6 C's)	

Each of these molecules could be used as an adjective to describe a group; for example, the top one where the R is not defined we could say that the defined parts are an isopropyl group. It's three carbons (propane) in the shape of the iso group.

But before getting into the systematic nomenclature of Substituted Alkanes: non-IUPAC names based on total number of C atoms present and position of functional group

Degree of Substitution



Nomenclature of Alkanes: IUPAC Names based on the number of C's in the longest continuous chain of C atoms

methane	CH ₄	
ethane	CH ₃ CH ₃	
propane	CH ₃ CH ₂ CH ₃	
butane	CH ₃ CH ₂ CH ₂ CH ₃	
pentane	CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	
hexane	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	
heptane	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	
octane	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	
nonane	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	
decane	CH ₃ CH ₂ CH ₃	
undecane	CH ₃ CH ₂	
dodecane	CH ₃ CH ₂	

Nomenclature of Alkanes: IUPAC Names based on the number of C's in the longest continuous chain of C atoms

Determine longest continuous chain.

- This is the **parent hydrocarbon**
- If compound has two or more chains of the same length, parent hydrocarbon is chain with greatest number of substituents

List the name of substituent(s) before the name of the parent hydrocarbon along with the number of the carbon to which it is attached--Substituents are listed in alphabetical order – neglecting prefixes such as di- tri- tert- etc.

- Find and list all of the substituents
- Names of alkyl substituents are based on the length of the substituent.
- Names for branched substituent such as *sec*-butyl and *tert*-butyl are acceptable, but systematic substituent names are preferable.
 - **o** The numbering system for a branched substituent begins with the carbon attached to the parent hydrocarbon
 - **o** This number together with the substituent name is placed inside parentheses
- Number the substituents
 - **o** in the direction that gives the lower number for the lowest-numbered substituent. (Lowest possible number for all substituents on the parent chain)
 - When both directions yield the same lower number for the lowest numbered substituent, select the direction that yields the lower number for the next lowest numbered substituent
 - If same substituent numbers are obtained in either direction, number in the direction giving lowest number to the first (alphabetically) named substituent

Form of name: #-followed by substituent name followed by parent hydrocarbon name

Nomenclature of Alkanes



(17) **Today**

Section 3.4 Nomenclature

Section 3.5 - 3.7 Properties and Conformations of Alkanes

(19) Second Class from Today

Chap 4 Cycloalkanes

Next Class (18)

Section 3.5 - 3.7 Properties and Conformations of Alkanes

Chap 4 Cycloalkanes

Third Class from Today (20)

Chap 4 Cycloalkanes

Reworked Test 1's due Wednesday Oct. 23.

On a separate piece of paper provide answers for any question for which you did not receive full credits. I do NOT need the test itself back.

longest chain:	
parent alkane name:	
functional group (?) and position:	
substituent names:	
substituent positions:	



Nomenclature of Alkanes

longest chain:	CH ₃ CH ₂ CHCH ₂ CH ₂ CH ₃
parent alkane name:	I CH ₃
functional group (?) and position:	
	name:
substituent names:	
substituent positions:	

Nomenclature of Alkanes

 $CH_{2}CH_{3}$ | $CH_{3}CH_{2}CHCH_{2}CHCH_{3}$ | CH_{3} longest chain: parent alkane name: functional group (?) and position: name: substituent names: substituent positions:

longest chain:	
parent alkane name:	
functional group (?) and position:	
substituent names:	
substituent positions:	

longest chain:	
parent alkane name:	
functional group (?) and position:	
substituent names:	
substituent positions:	

Isomers



(18) **Today**

Section 3.5 - 3.7 Conformations of Alkanes

Next Class (19)

Section 3.5 - 3.7 Conformations of Alkanes

Chap 4 Cycloalkanes Section 4.1 Naming Cycloalkanes and Halogen Substituents

Section 4.2 cis-trans isomerism

(20) Second Class from Today

Section 4.2 cis-trans isomerism

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Third Class from Today (21)

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Sections 5.1 – 5.5 Chirality and Determining the Configuration of Chiral Centers



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





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

T



Strain Energy as a Function of C-2 to C-3 Dihedral Angle in Butane



Showing 3-D Relationships (stereochemistry) Using Newman Projections

Drawn as though one is looking along a bond

Front carbon is a where three bonds come together

Back carbon is a large circle





Practice Using Newman Projections

Draw the Newman projection along the C_2 to C_3 bond in the following structure



Draw the Newman projection along the C₃ to C₂ bond in the following structure



Practice Using Newman Projections

Draw the Newman projection along the C₂ to C₃ bond in the following structure



Practice Using Newman Projections

Draw the Newman projection along the C₂ to C₃ bond in the following structure


Practice Using Newman Projections

Sections 3.6 - 3.7

Draw the Newman projection along the C₃ to C₂ bond in the following structure

Practice Using Newman Projections

Draw the Newman projection along the C₃ to C₂ bond in the following structure



(19) **Today**

3.6 - 3.7 Practicing Newman Projections

Chap 4 Cycloalkanes Section 4.1 Naming Cycloalkanes and Halogen Substituents

Section 4.2 cis-trans isomerism

(21) Second Class from Today

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Section 4.2 cis-trans isomerism

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Third Class from Today (22)

Chap 5

Next Class (20)