

Organic Chemistry

GV: Lê Quốc Chơn

My background:

Chemical engineer: Da Nang University of Technology (Viet Nam)
Master in Physical Chemistry: Uni Paris Sud – 11 (France)
Ph.D. in Physical Chemistry of Materials: Uni Nantes (France)
Postdoctoral researcher: Uni Laval (Québec – Canada).

Liên lạc:

0931.383.074

lequocchon@gmail.com

Địa điểm: Phòng 707, Khoa Tự Nhiên, 03 Quang Trung



Write on your paper and give it to me. NOW

About yourself

1. Your Chemistry grade at high school
2. Điểm thi đại học bao nhiêu?
3. Your career plan?
4. Is Chemistry important to you? Why?
5. What do you want to learn in this course?
6. How do you learn Chemistry?
7. Các khái niệm hóa học khó hiểu/chưa hiểu?

One more slide



Answer these questions

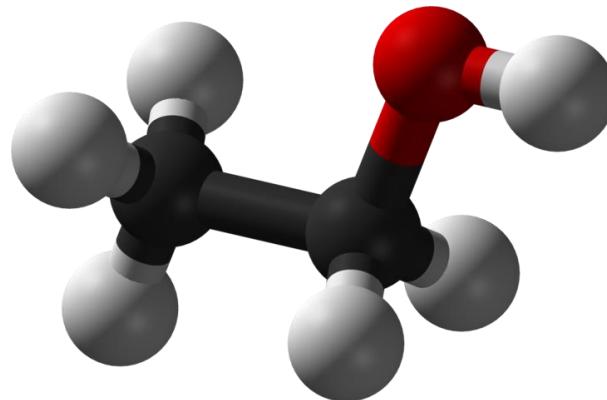
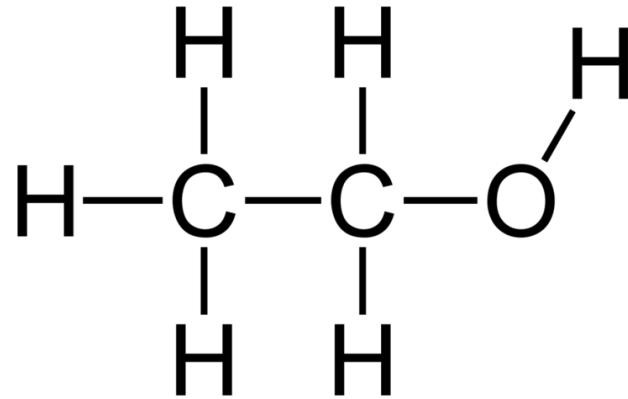
- Draw structure of ethanol, acetic acid, butane and propane.
- Name 5 functional groups that you know.
- Name different chemical bonds that you know.
- Name 5 chemical compounds that you know.

Write on your paper and give it to me!



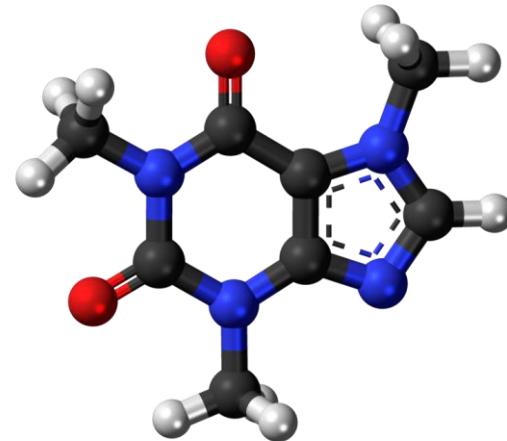
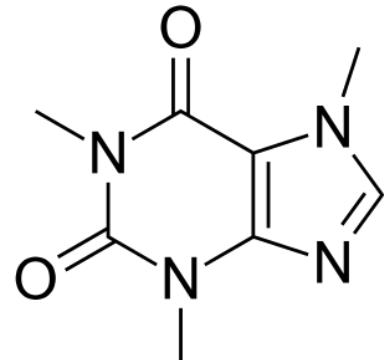
Background test

- Ethanol?



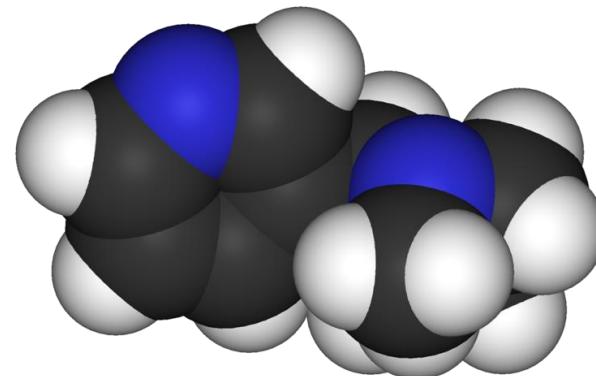
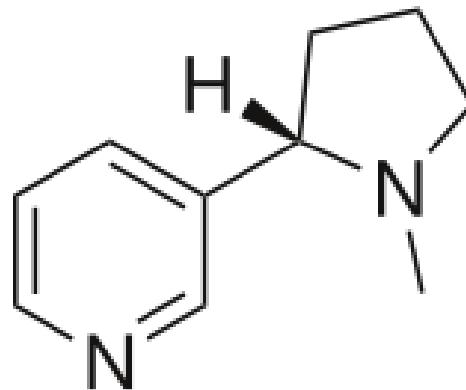
Background test

- Caffeine?



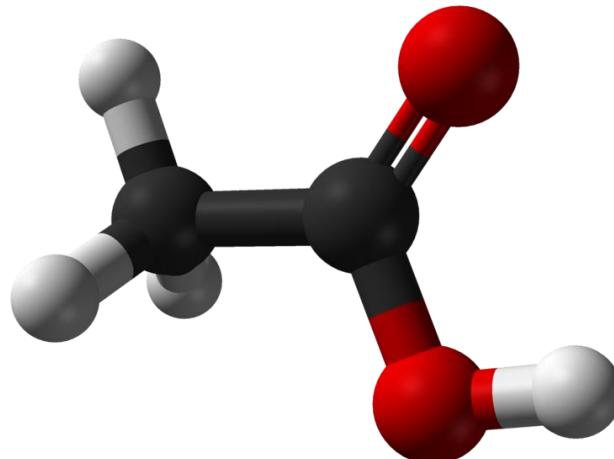
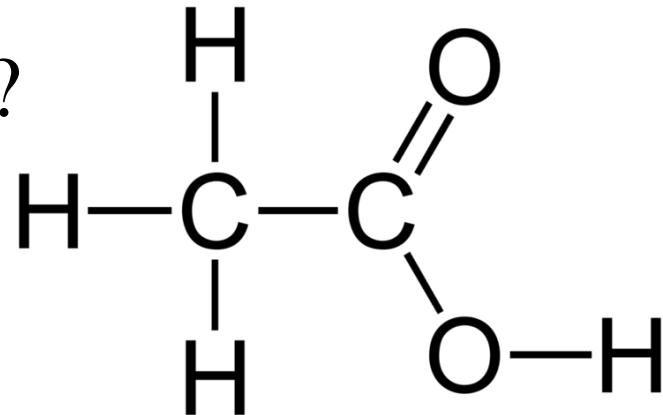
Background test

- Nicotine?

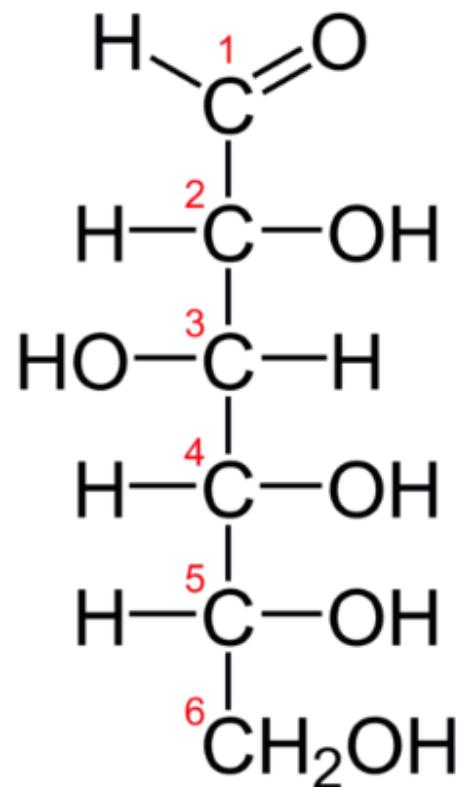


Background test

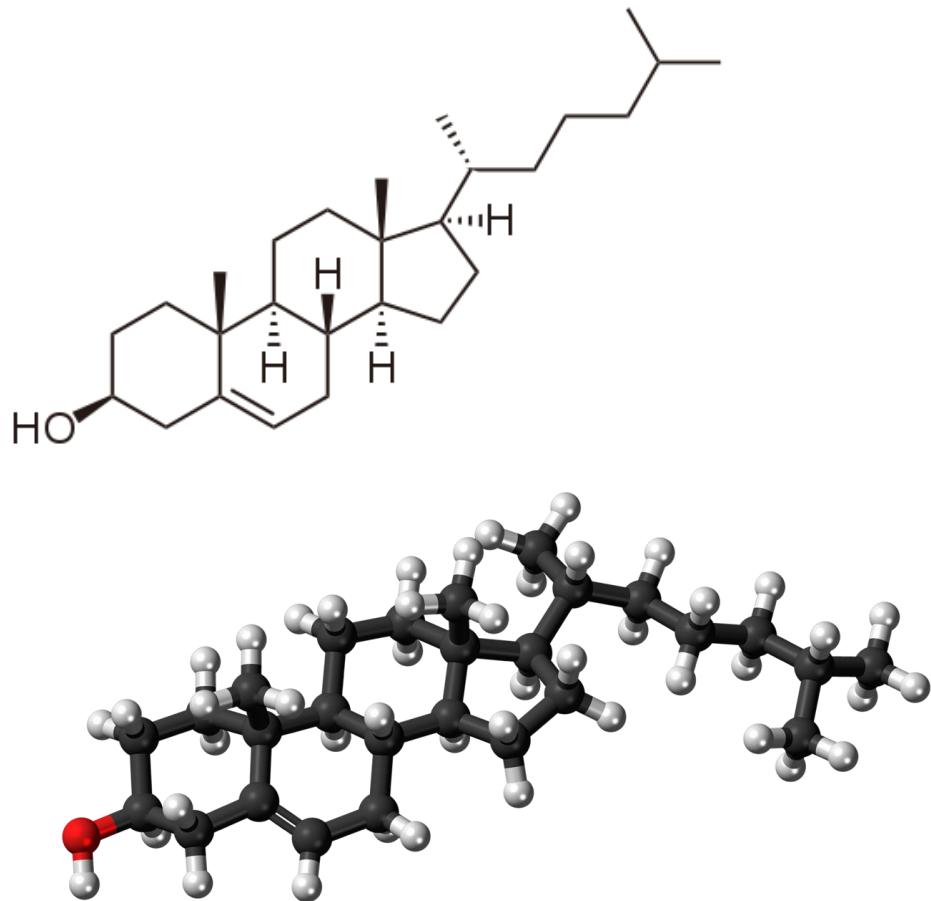
- Acid in Vinegar?



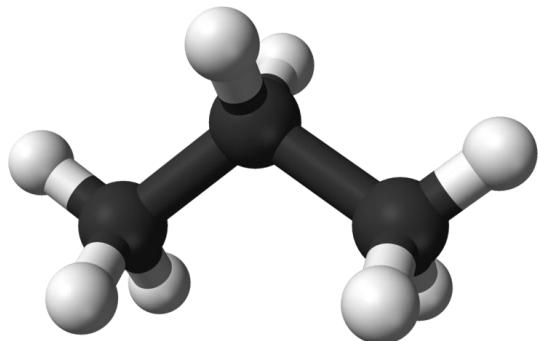
D-Glucose



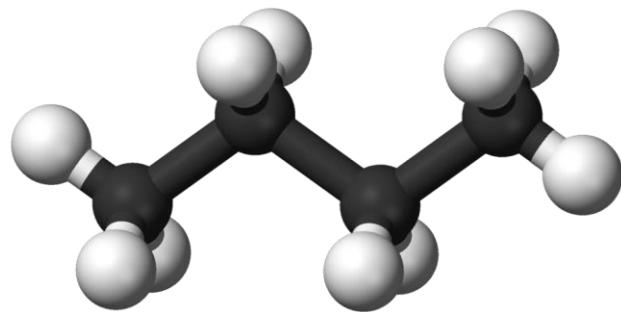
Cholesterol



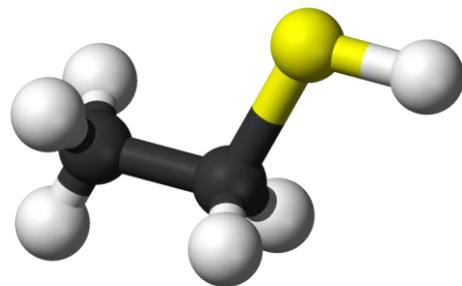
Liquefied petroleum gas (LPG)



propane



butane



(ethanethiol
or methyl captan)

Phân bổ điểm

TÊN LỚP: CHE 203 F HÓA HỮU CƠ

Chọn Quy tắc Tính
điểm

Chuyên Cần

Quy Tắc Tính Điểm của Đại Học Duy Tân (từ)

Phát Biểu & Thảo Luận

10.00 (0.00 - 20.00%) Còn lại: 10.00% [Cu thể Bài qiao](#)

Kiểm Tra Thường Kỳ

5.00 (0.00 - 20.00%) Còn lại: 5.00% [Cu thể Bài qiao](#)

Bài Tập Về Nhà

15.00 (0.00 - 30.00%) Còn lại: 15.00% [Cu thể Bài qiao](#)

Thực Hành & Thực Tế

0.00 (0.00 - 25.00%) Còn lại: 0.00%

Kiểm Tra Giữa Kỳ

0.00 (0.00 - 25.00%) Còn lại: 0.00%

Đồ Án Cá Nhân

0.00 (0.00 - 15.00%) Còn lại: 0.00%

Đồ Án Nhóm

15.00 (0.00 - 25.00%) Còn lại: 15.00% [Cu thể Bài qiao](#)

Kiểm Tra Cuối Kỳ

40.00 (20.00 - 55.00%) Còn lại: 40.00% [Cu thể Bài qiao](#)

TỔNG

100.00 (100%)

Kiểm tra cuối kỳ: Trắc nghiệm trên PC

Điều kiện Tổng theo Cụm:

0.00% ≤ Chuyên Cần + Phát Biểu & Thảo Luận ≤ 20.00%

0.00% ≤ Kiểm Tra Thường Kỳ + Bài Tập Về Nhà ≤ 30.00%

Đồ Án Cá Nhân + Đồ Án Nhóm + Kiểm Tra Cuối Kỳ = 55.00%



Textbooks

- McMurry, Organic Chemistry 9th - Brook Cole 2015
- Daniel P. Weeks-Pushing Electrons-Cengage Learning 2013
- Graham Solomons, Organic Chemistry, 11^{ed}, Wiley 2014
- Giáo trình Hóa Hữu Cơ – (GV. Nguyễn Văn Tiến) - DTU

Software

Avogadro (free) and Gaussian 09 (commercial)



Viết email ra sao?

lequocchon@gmail.com

New Message — ✉ ✕

To LE Quoc Chon <lequocchon@gmail.com> Cc Bcc

Subject 2019CHE203L_hoten_ chủ đề

Chào Thầy,

Em tên là Thích Hữu Cơ, lớp CHE203L. Em viết mail báo với Thầy là em rất ghiền môn Hóa Hữu Cơ và sẽ học giỏi môn này.

Em chúc Thầy khỏe và cho tụi em nhiều bài khó, và hay hơn nữa.

Thích Hữu Cơ



<http://lequocchon.blogspot.com/>

Le Quoc Chon blog

Home

About me

Mythought

VnScience

VnEducation

VnLife

News sites

Monday, December 25, 2017

Cái ích của học tập

Posted by LE Quoc Chon at 9:22 PM

No comments:



Thursday, December 21, 2017

Hướng dẫn Học Hóa Hữu Cơ

Posted by LE Quoc Chon at 9:33 PM

No comments:



►

Blog Archive

▼ 2017 (34)

▼ December (4)

Cái ích của học tập

Hướng dẫn Học Hóa Hữu Cơ

Can đảm đối diện với thế giới

Việt Nam nên đầu tư thêm nỗ

Dục Đại Học

► September (5)

► August (4)

► June (1)

► May (2)



Lecture 1: Structure and bonding

Cấu trúc và liên kết



Milky Way Galaxy

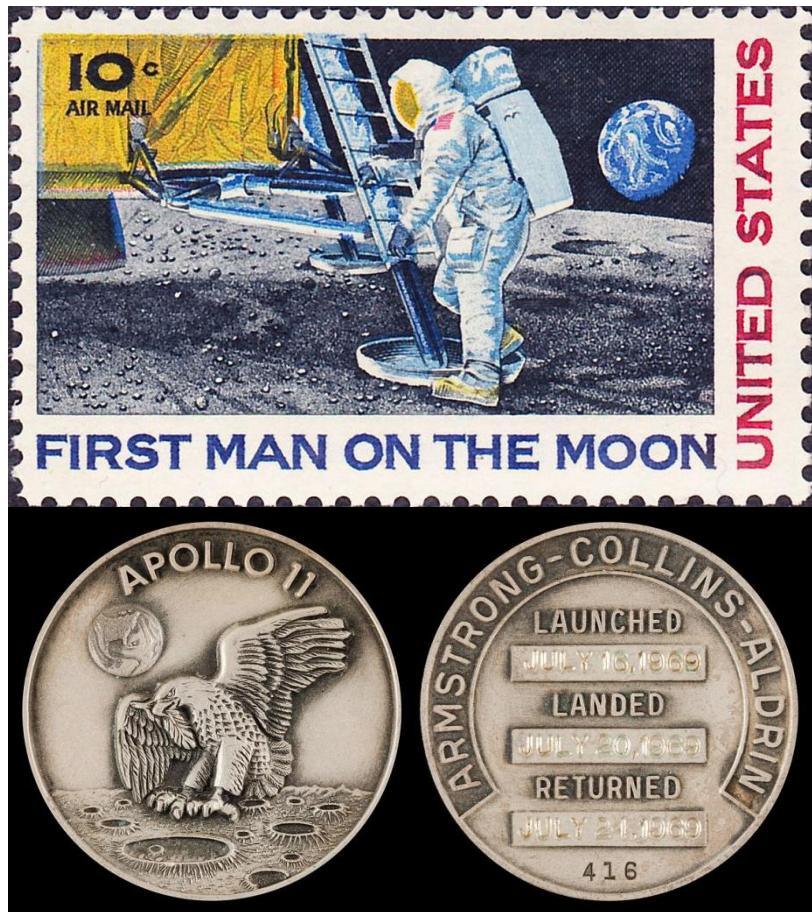
Most Known
Exoplanets

Our Solar System

Newfound Exoplanet

Matter & Energy
 $E = mc^2$

Curiosity about Nature!

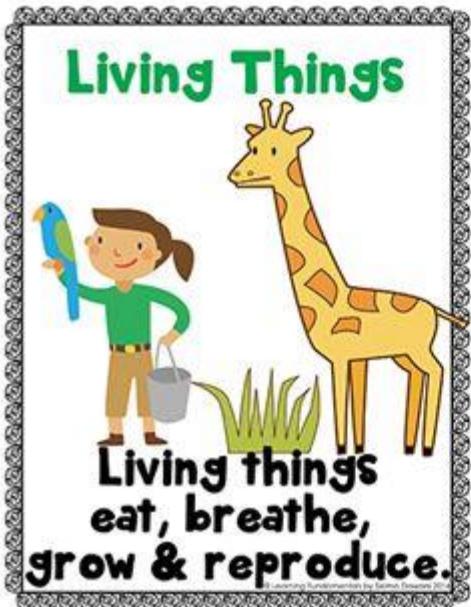


Physics – **Chemistry** - Biology

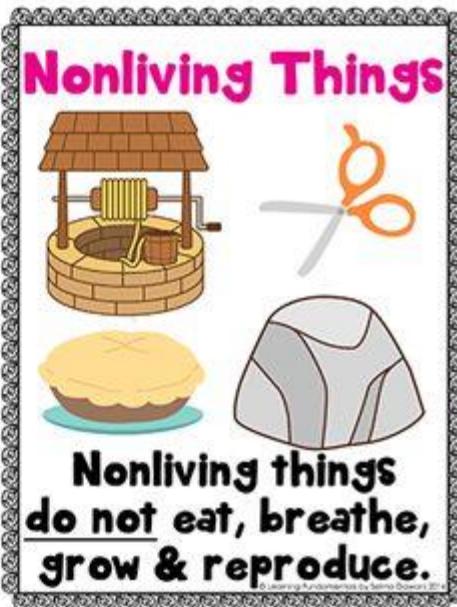


Chemistry

Organic



Inorganic



A pallasite: stony-iron meteorite

Scientifically, no barrier!

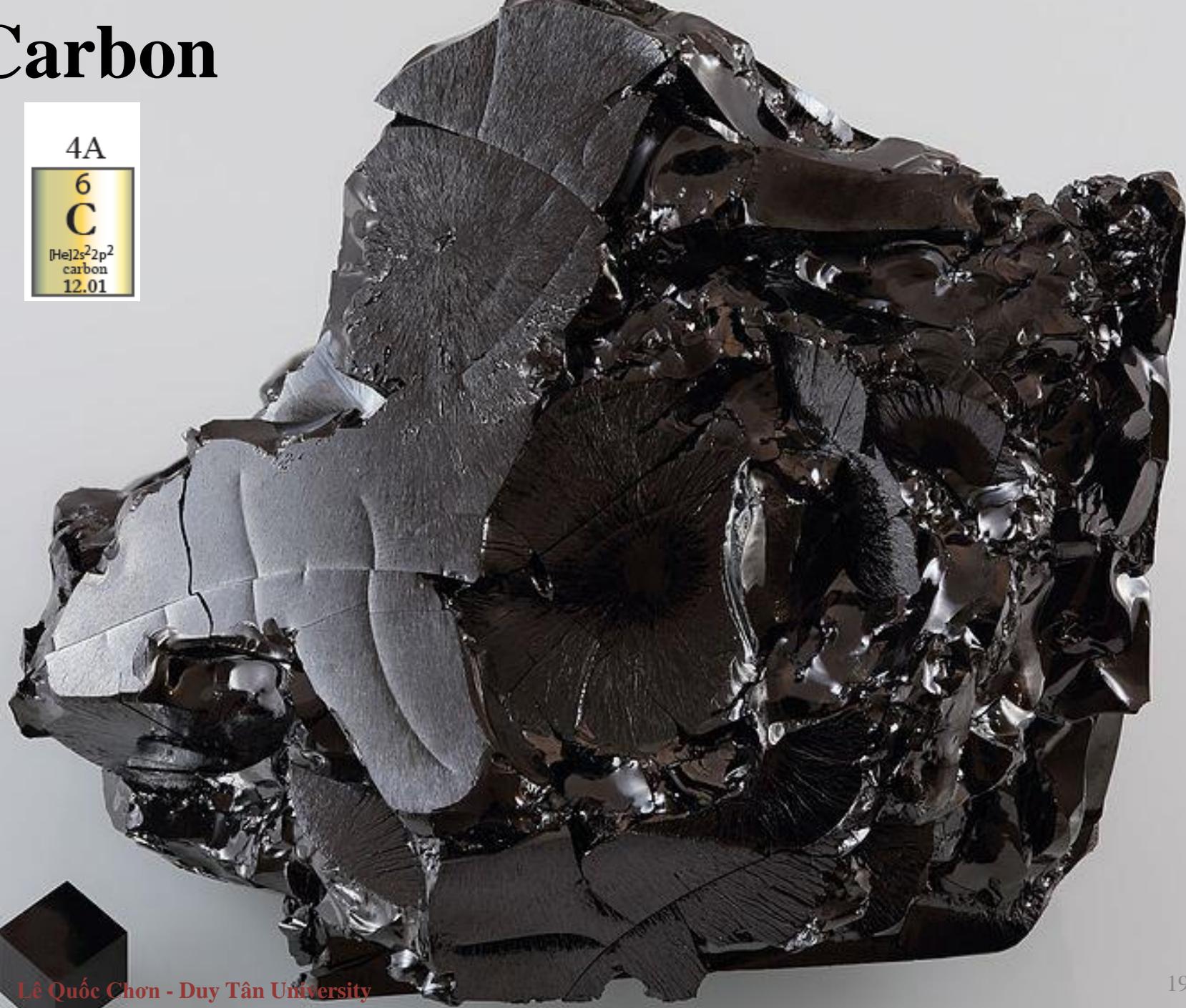


Carbon

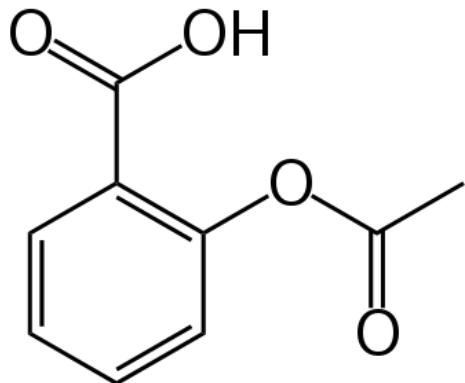
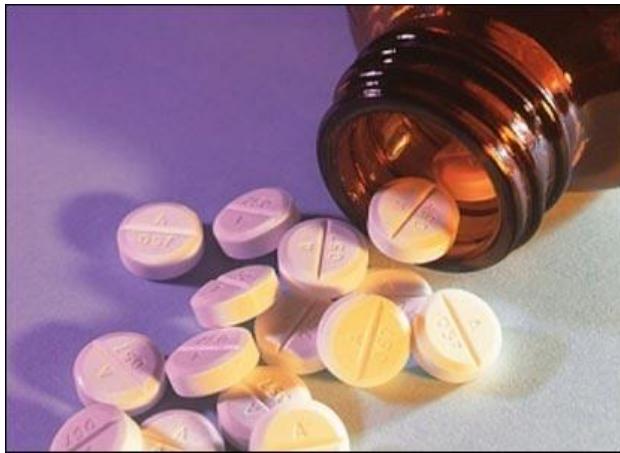
4A

6
C

[He]2s²2p²
carbon
12.01

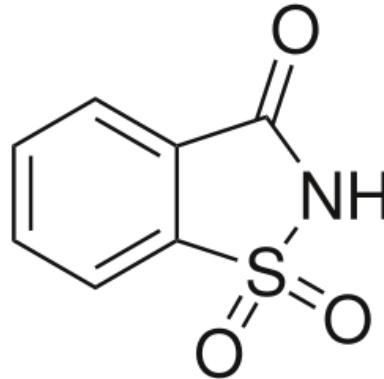


Organic chemistry: applications



Aspirin

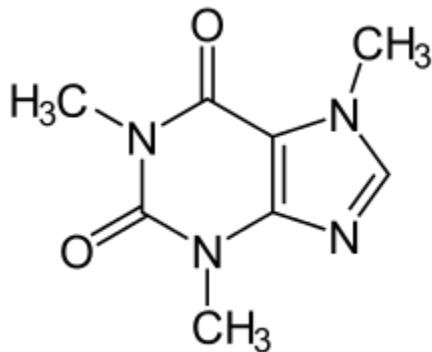
1853 by Charles Frédéric Gerhardt



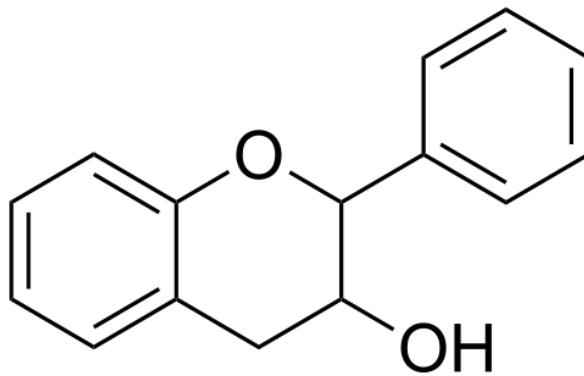
Saccharin
artificial sweetener
synthesized 1879

• • •

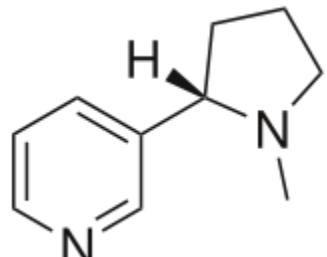
Today: > 50 millions compounds



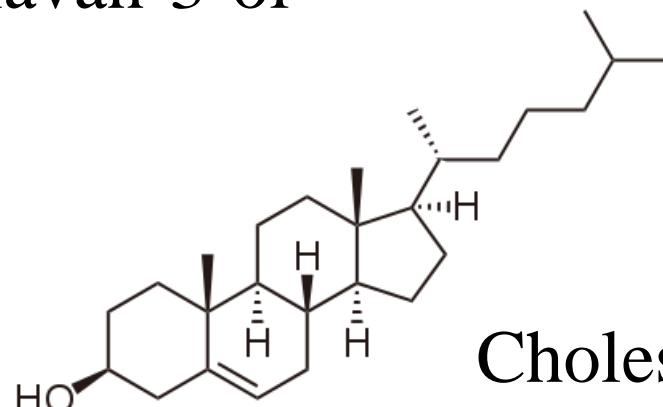
Caffeine



Flavan-3-ol



Nicotine



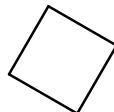
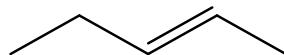
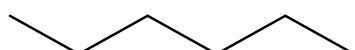
Cholesterol



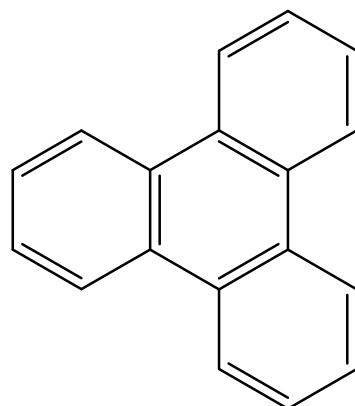
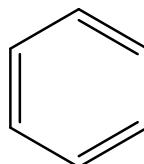
Classification

Phân loại

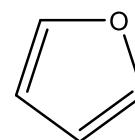
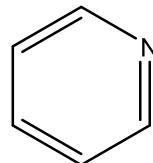
Aliphatic



Aromatic



Heterocyclic



Polymers

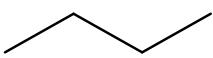
Biomolecules



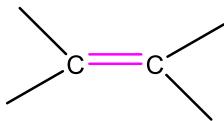
Classification

Functional groups (theo nhóm chức)

alkane



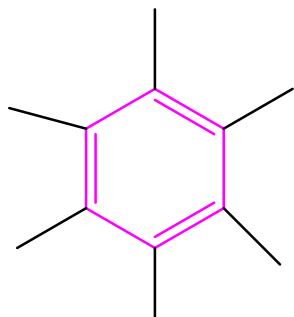
alkene



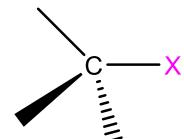
alkyne



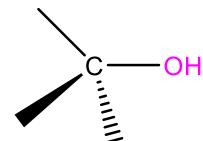
arene



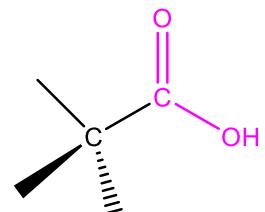
halide



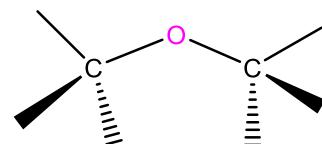
alcohol



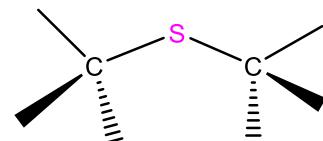
carboxylic acid



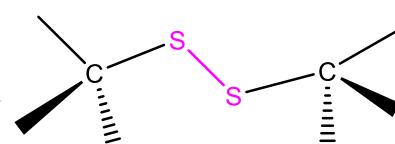
ether



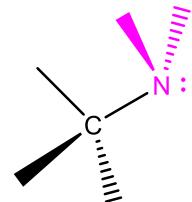
sulfide



disulfide



amine



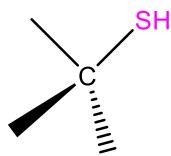
Classification

Functional groups

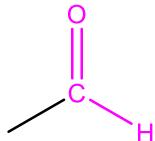
nitrile



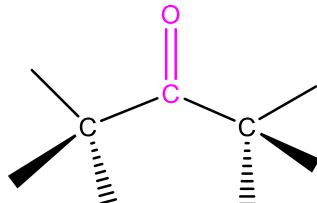
thiol



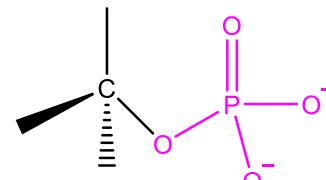
aldehyde



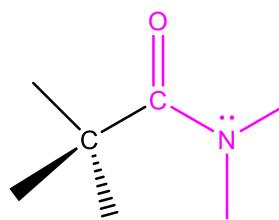
ketone



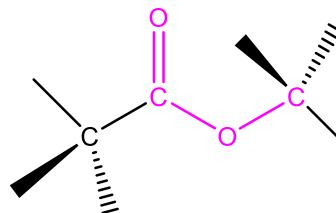
phosphate



amide



ester



Một số từ khóa trong Hóa Hữu Cơ

Organic Chemistry

molecule

structure

reactivity

bond

mechanism

atom

synthesis

electron

orbital

making bond & breaking bond

nucleophile & electrophile

computational chemistry

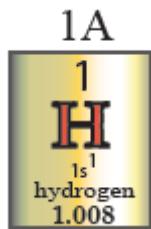
& beyond

Arts & sciences !



Structure and bonding

Cấu trúc và liên kết



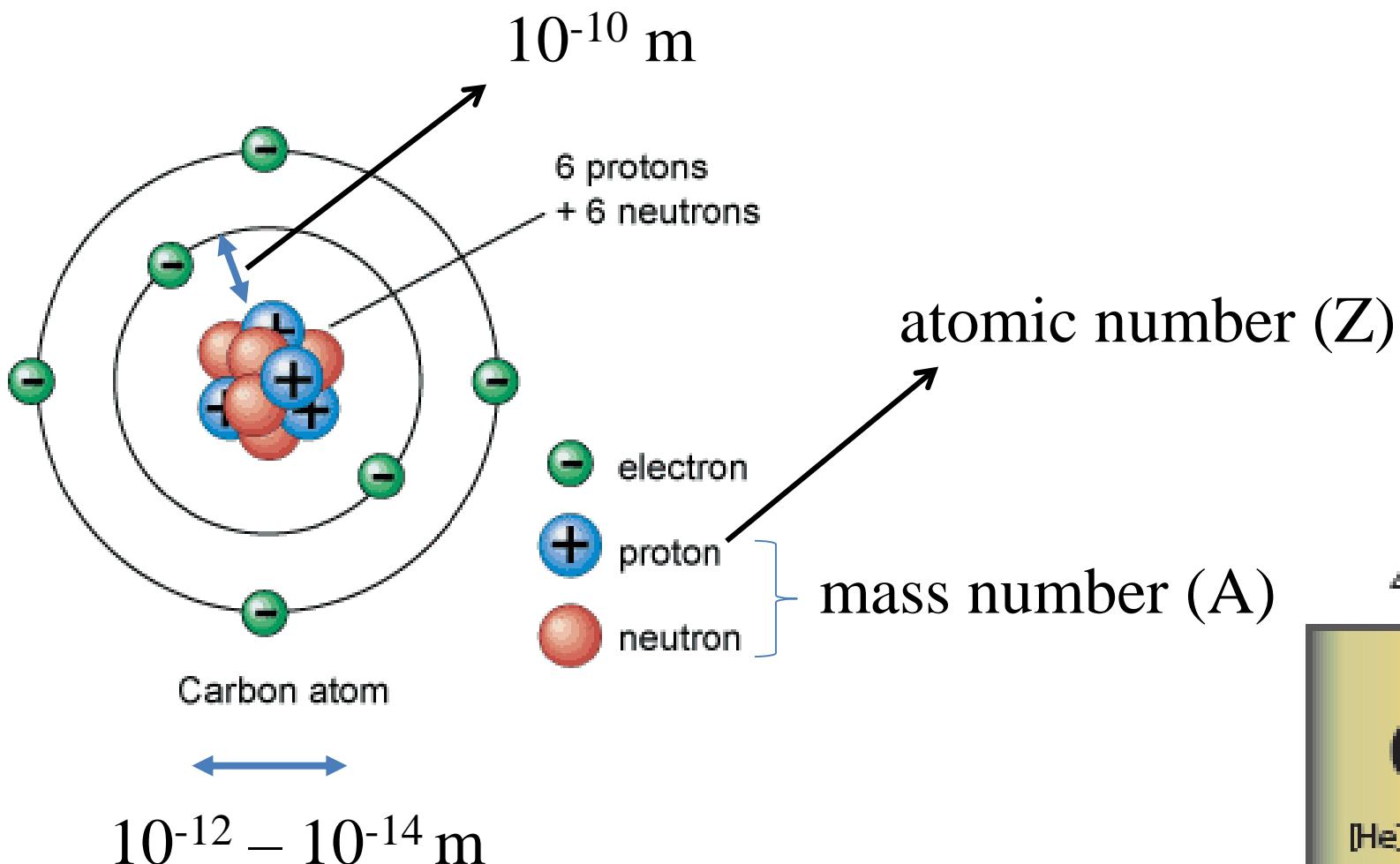
3A	4A	5A	6A	7A
5 B [He]2s ² 2p ¹ boron 10.81	6 C [He]2s ² 2p ² carbon 12.01	7 N [He]2s ² 2p ³ nitrogen 14.01	8 O [He]2s ² 2p ⁴ oxygen 16.00	9 F [He]2s ² 2p ⁵ fluorine 19.00
13 Al [Ne]3s ² 3p ¹ aluminum 26.98	14 Si [Ne]3s ² 3p ² silicon 28.09	15 P [Ne]3s ² 3p ³ phosphorus 30.97	16 S [Ne]3s ² 3p ⁴ sulfur 32.06	17 Cl [Ne]3s ² 3p ⁵ chlorine 35.45
				35 Br [Ar]4s ² 3d ¹⁰ 4p ⁵ bromine 79.90
				53 I [Kr]5s ² 4d ¹⁰ 5p ⁵ iodine 126.9

Key concepts (khái niệm chính trong bài này)

- Nucleus & electron
- Electron configuration
- Valence bond theory
- Orbital hybridization
- Molecular orbital theory
- Drawing chemical structure



Nucleus & electron



Orbitals



3rd shell
(capacity—18 electrons)

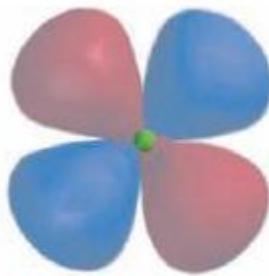
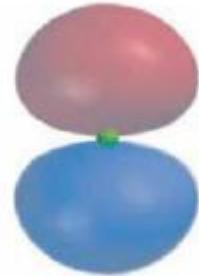
<i>3d</i>	↑↓	↑↓	↑↓	↑↓	↑↓
<i>3p</i>	↑↓	↑↓	↑↓		
<i>3s</i>	↑↓				

2nd shell
(capacity—8 electrons)

<i>2p</i>	↑↓	↑↓	↑↓
<i>2s</i>	↑↓		

1st shell
(capacity—2 electrons)

<i>1s</i>	↑↓
-----------	----



s orbital

p orbital

d orbital



<i>2p</i>	↑	↑	—
<i>2s</i>	↑↓		
<i>1s</i>	↑↓		

at ground state

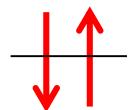
Electron configuration

Cấu hình electron

Orbital filling according to order:

1s 2s 2p 3s 3p 4s 3d

Electron has spin with 2 directions: up & down
An orbital contains maximum 2 electrons



Electrons tend to occupy orbital to get maximum number of parallel spin direction.

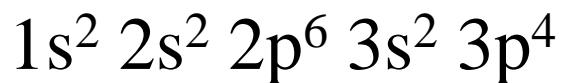
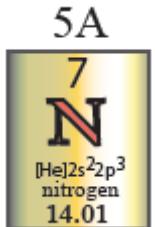
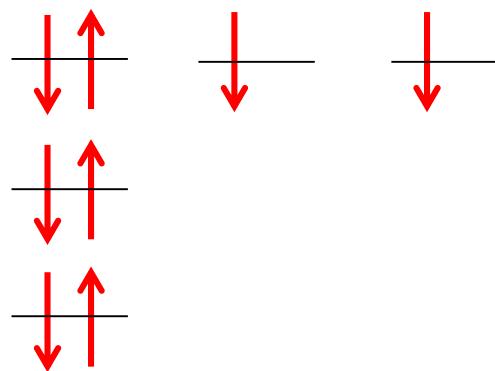
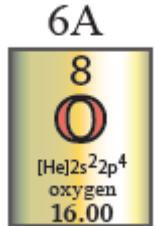
Phosphorus (P)
with 15 electrons

3p	↑	↑	↑
3s	↑↓		
2p	↑↓	↑↓	↑↓
2s	↑↓		
1s	↑↓		



Problem 1.1

Write the electron configuration of O, N and S at ground-state?



Problem 1.2

How many electrons does each of the following element have in its outer-most electron shell? Mg, Co, Se



PERIODIC TABLE

Atomic Properties of the Elements

Group
1
IA

1	^{2S_{1/2}} H Hydrogen 1.00794 1s 13.9894	2	IIA
3	^{2S_{1/2}} Li Lithium 6.941 1s ² 5.3917	4	^{1S₀} Be Beryllium 9.012182 1s ² s ² 9.3227
11	^{2S_{1/2}} Na Sodium 22.98976928 [Ne]3s 5.1391	12	^{1S₀} Mg Magnesium 24.3050 [Ne]3s ² 7.6462

Period

19	^{2S_{1/2}} K Potassium 39.0983 [Ar]4s 4.3407
20	^{1S₀} Ca Calcium 40.078 [Ar]3d ^{4s²} 6.1132

21	^{2D_{3/2}} Sc Scandium 44.955912 [Ar]3d ^{4s²} 6.5615
22	^{3F₂} Ti Titanium 47.867 [Ar]3d ^{4s²} 6.7462

23	^{4F_{3/2}} V Vanadium 50.9415 [Ar]3d ^{4s²} 6.7665
24	^{7S₃} Cr Chromium 51.9961 [Ar]3d ^{4s²} 7.3430

25	^{6S_{5/2}} Mn Manganese 54.938045 [Ar]3d ^{4s²} 7.9024
26	^{5D₄} Fe Iron 55.845 [Ar]3d ^{4s²} 7.9024

27	^{4F_{9/2}} Co Cobalt 58.933195 [Ar]3d ^{4s²} 7.8810
28	^{3F₄} Ni Nickel 58.6934 [Ar]3d ^{4s²} 7.6399

29	^{2S_{1/2}} Cu Copper 63.546 [Ar]3d ^{4s²} 7.7264
30	^{1S₀} Zn Zinc 65.38 [Ar]3d ¹⁰ 9.3942

31	^{2P^o} Ga Gallium 69.723 [Ar]3d ¹⁰ 9.5993
32	^{3P^o} Ge Germanium 72.64 [Ar]3d ¹⁰ 9.7894

33	^{4S_{3/2}} As Arsenic 74.92160 [Ar]3d ¹⁰ 9.7524
34	^{3P₂} Se Selenium 78.96 [Ar]3d ¹⁰ 9.0096

35	^{2P_{3/2}} Br Bromine 79.904 [Ar]3d ¹⁰ 11.1838
36	^{1S₀} Kr Krypton 83.798 [Ar]3d ¹⁰ 13.9996

37	^{2S_{1/2}} Rb Rubidium 85.4678 [Kr]5s 4.1771
38	^{1S₀} Sr Strontium 87.62 [Kr]5s ² 5.6949

39	^{2D_{3/2}} Y Yttrium 88.90585 [Kr]4d ^{5s²} 6.2173
40	^{3F₂} Zr Zirconium 91.224 [Kr]4d ^{5s²} 6.6339

41	^{6D_{1/2}} Nb Niobium 95.96 [Kr]4d ^{5s²} 7.0924
42	^{7S₃} Mo Molybdenum 95.96 [Kr]4d ^{5s²} 7.2835

43	^{6S_{5/2}} Tc Technetium (98) [Kr]4d ^{5s²} 7.28
44	^{5F₅} Ru Ruthenium 101.07 [Kr]4d ^{5s²} 7.3605

45	^{4F_{9/2}} Rh Rhodium 102.90550 [Kr]4d ^{5s²} 7.4589
46	^{1S₀} Pd Palladium 106.42 [Kr]4d ¹⁰ 8.9369

47	^{2S_{1/2}} Ag Silver 107.8682 [Kr]4d ¹⁰ 8.9938
48	^{1S₀} Cd Cadmium 112.411 [Kr]4d ¹⁰ 9.5762

49	^{2P^o} Tl Thallium 200.59 [Xe]4f ¹⁴ 10.4375
50	^{3P^o} In Indium 114.818 [Xe]4f ¹⁴ 9.74167

51	^{4S_{3/2}} Sb Antimony 121.760 [Xe]4f ¹⁴ 8.6084
52	^{3P₂} Te Tellurium 127.60 [Xe]4f ¹⁴ 9.0096

53	^{2P^o} I Iodine 126.90447 [Xe]4f ¹⁴ 10.4513
54	^{1S₀} Xe Xenon 131.293 [Kr]4d ¹⁰ 12.1298

55	^{2S_{1/2}} Cs Cesium 132.9054519 [Xe]6s 3.8939
56	^{1S₀} Ba Barium 137.327 [Xe]6s ² 5.2117

57	^{2D_{3/2}} La Lanthanum 138.90547 [Xe]5d ^{6s²} 5.5769
58	^{1G₄} Ce Cerium 140.116 [Xe]4f ^{6d^{6s²}} 5.5387

59	^{4I_{9/2}} Pr Praseodymium 140.90765 [Xe]4f ⁷ 5.473
60	^{5I₄} Nd Neodymium 144.242 [Xe]4f ⁸ 5.5250

61	^{6H_{5/2}} Pm Promethium (145) [Xe]4f ⁸ 5.582
62	^{7F₀} Sm Samarium 150.36 [Xe]4f ⁸ 5.6437

63	^{8S_{7/2}} Eu Europium 151.964 [Xe]4f ⁸ 5.6704
64	^{9D₂} Gd Gadolinium 157.25 [Xe]4f ⁹ 5.6838

65	^{6H_{15/2}} Tb Terbium 158.92535 [Xe]4f ¹⁰ 5.6838
66	^{5I₈} Dy Dysprosium 162.500 [Xe]4f ¹¹ 6.0215

67	^{4I_{15/2}} Ho Holmium 164.93032 [Xe]4f ¹¹ 6.1077
68	^{3H₆} Er Erbium 167.259 [Xe]4f ¹¹ 6.2542

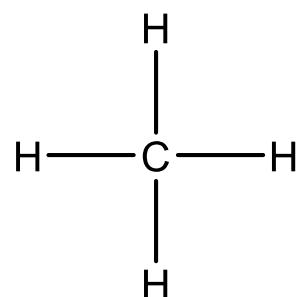
69	^{2F_{7/2}} Tm Thulium 173.054 [Xe]4f ¹⁴ 5.4259
70	^{1S₀} Yb Ytterbium 174.9668 [Xe]4f ¹⁴ 5.4259

71	^{2D_{3/2}} Lu Lutetium 174.9668 [Xe]4f ¹⁴ 5.4259
72	^{1S₀} He Helium 4.002602 1s ² 24.5874

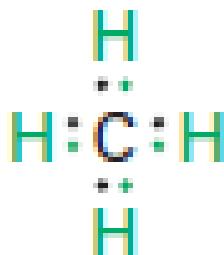
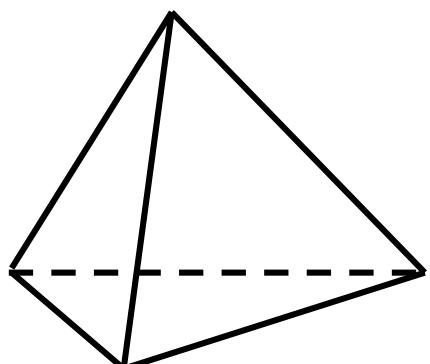
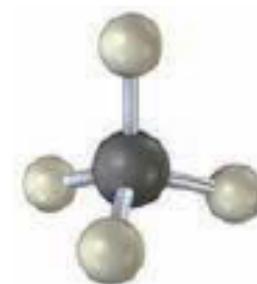
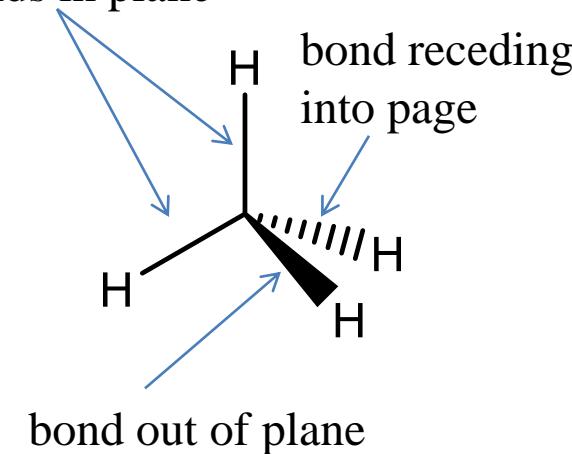
Frequently used fundamental physical constants													
For the most accurate values of these and other constants, visit physics.nist.gov/constants													
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³ Cs													
speed of light in vacuum													
c = 299 792 458 m s ⁻¹ (exact)													
Planck constant													
h = 6.6261 × 10 ⁻³⁴ J s (h = h/2π)													
elementary charge													

Chemical bond theory

Lý thuyết liên kết hóa học



bonds in plane

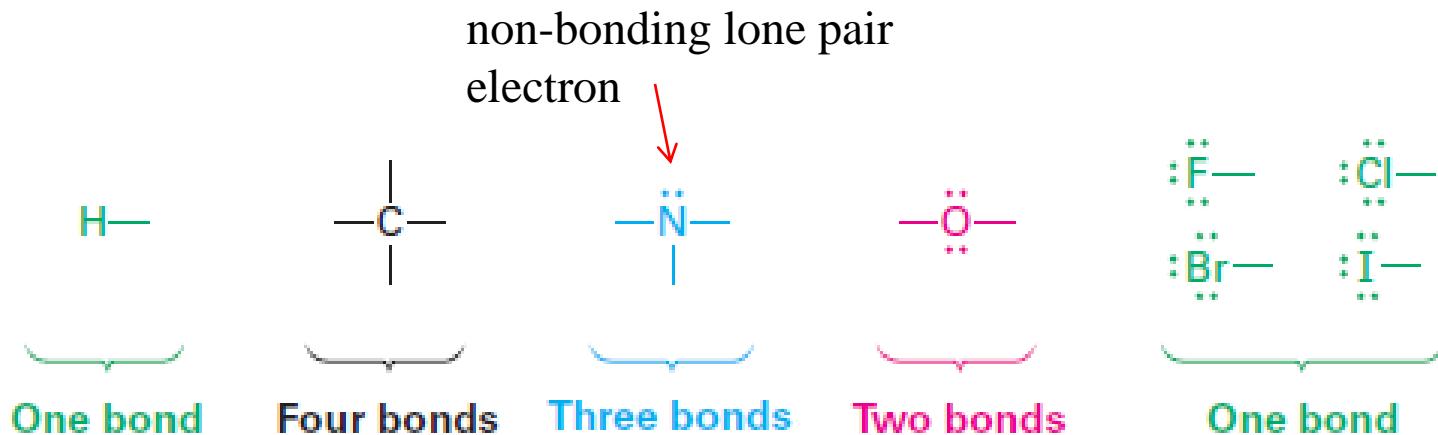


Lewis structure



Regular tetrahedron
Lê Quốc Chơn - Duy Tân University

Chemical bond theory



Công thức phân tử của phosphine là gì? PH_?

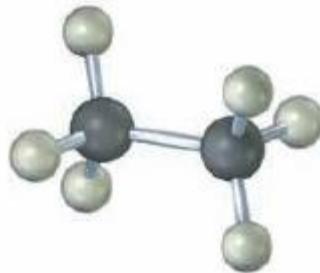
Vẽ cấu trúc của chloromethane CH₃Cl, dùng công thức Lewis



Problem 1.3 & 1.4

Show the tetrahedral geometry of chloroform CHCl_3 using solid, dashed and wedged lines?

And for ethane?



Problem 1.5,1.6 & 1.7

1.5. Guess the chemical formula of these substances: $\text{CCl}_?$, $\text{AlH}_?$, $\text{CH}_?\text{Cl}_2$, $\text{SiF}_?$, $\text{CH}_3\text{NH}_?$.

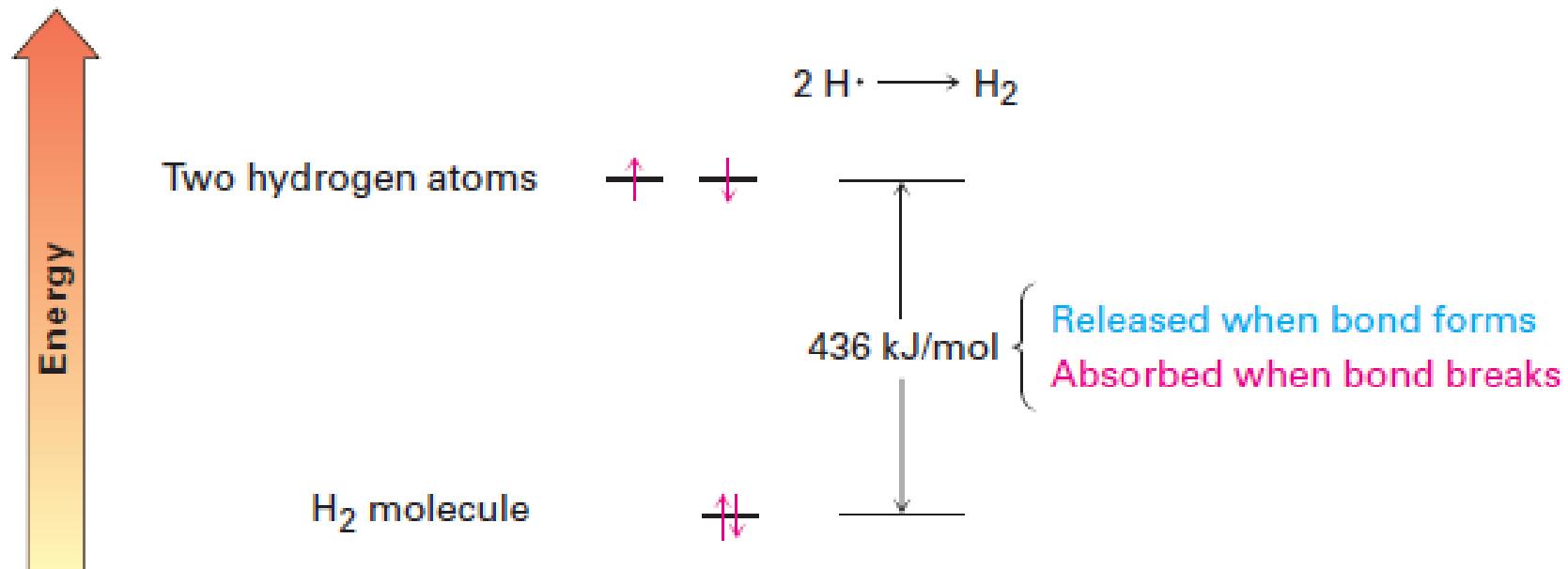
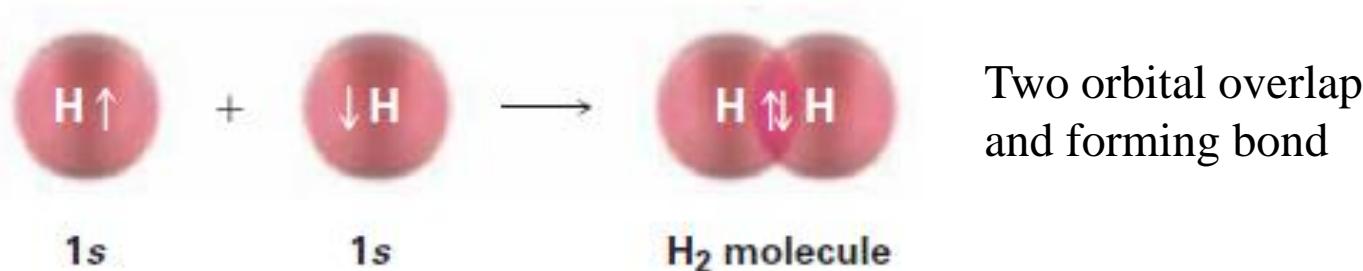
1.6. Write line-bond structures for the following substances, showing all non-bonding electrons:
 CHCl_3 , CH_3NH_2 , H_2S , CH_3Li

1.7. Does this formula exist in organic chemistry C_2H_7 ?



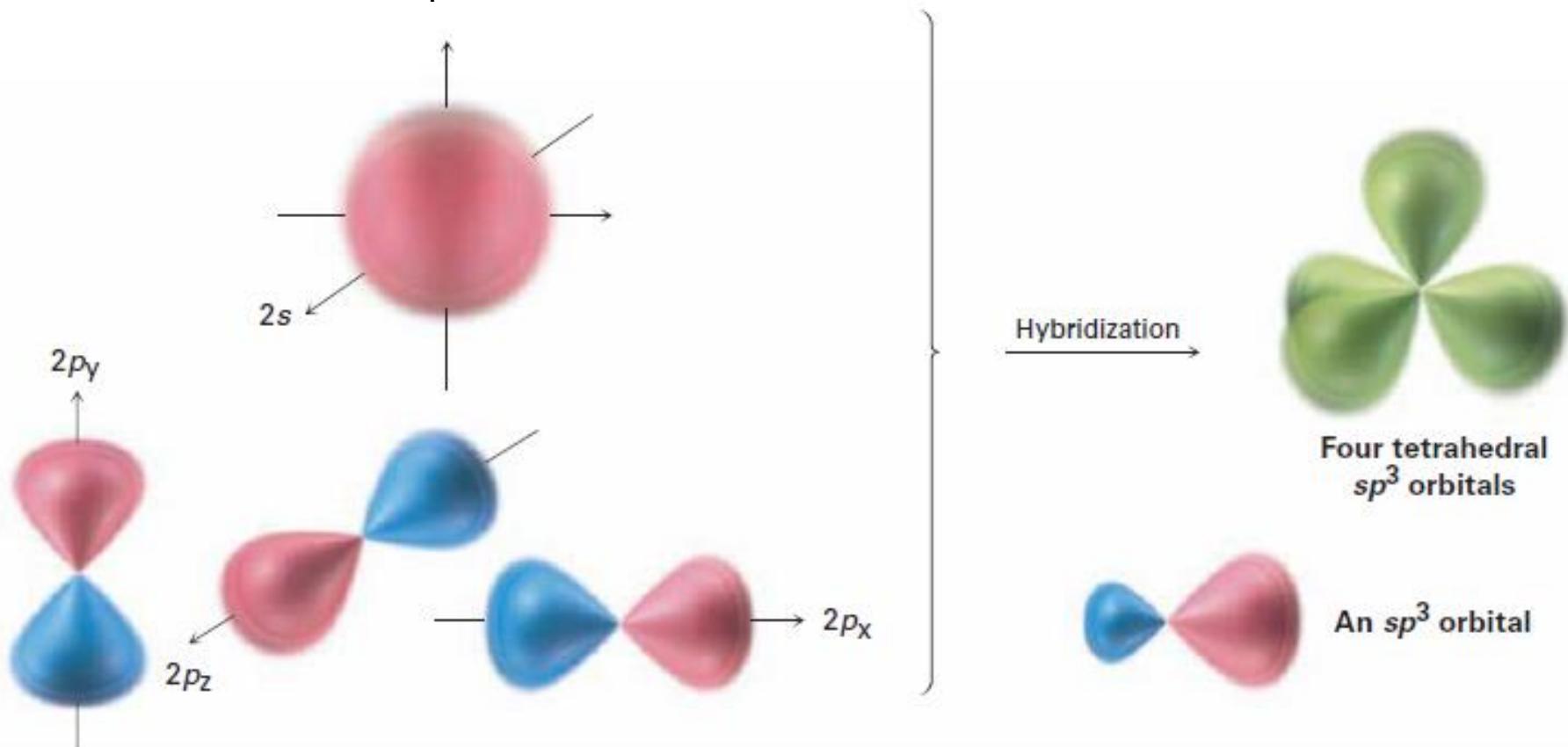
Valence bond theory

Thuyết liên kết cộng hóa trị

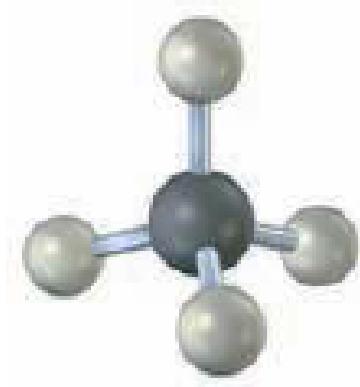
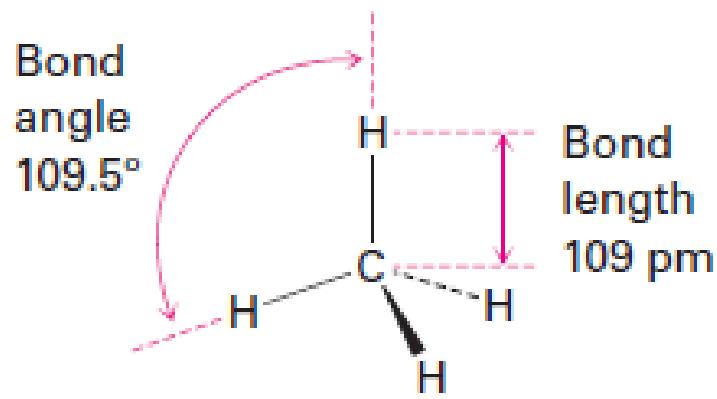


Valence bond theory: sp^3 hybridization Lai hóa sp^3

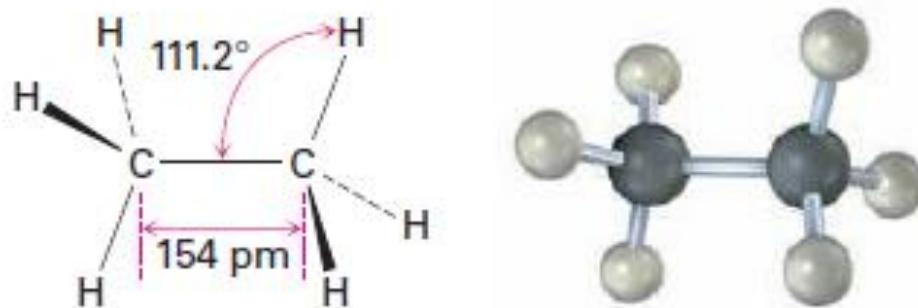
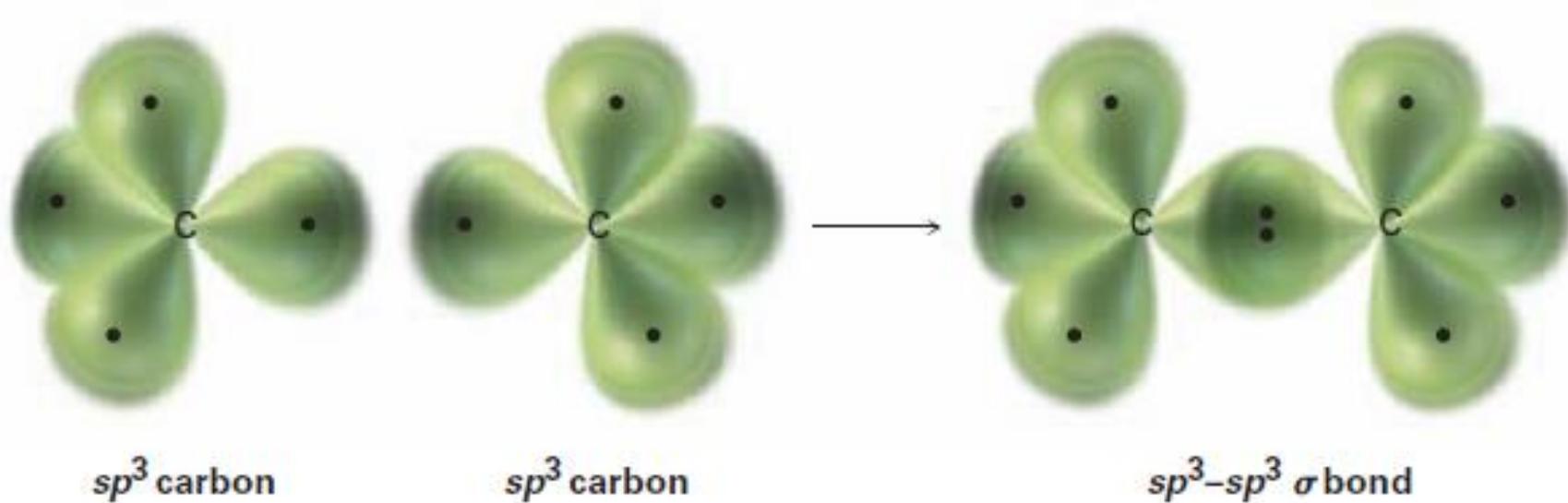
Methane: CH_4



Valence bond theory: sp^3 hybridization



Ethane: sp^3 hybridization



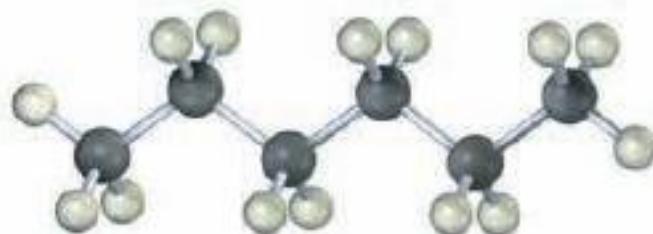
Problem 1.8

PROBLEM 1-8

Draw a line-bond structure for propane, $\text{CH}_3\text{CH}_2\text{CH}_3$. Predict the value of each bond angle, and indicate the overall shape of the molecule.

PROBLEM 1-9

Convert the following molecular model of hexane, a component of gasoline, into a line-bond structure (gray = C, ivory = H).

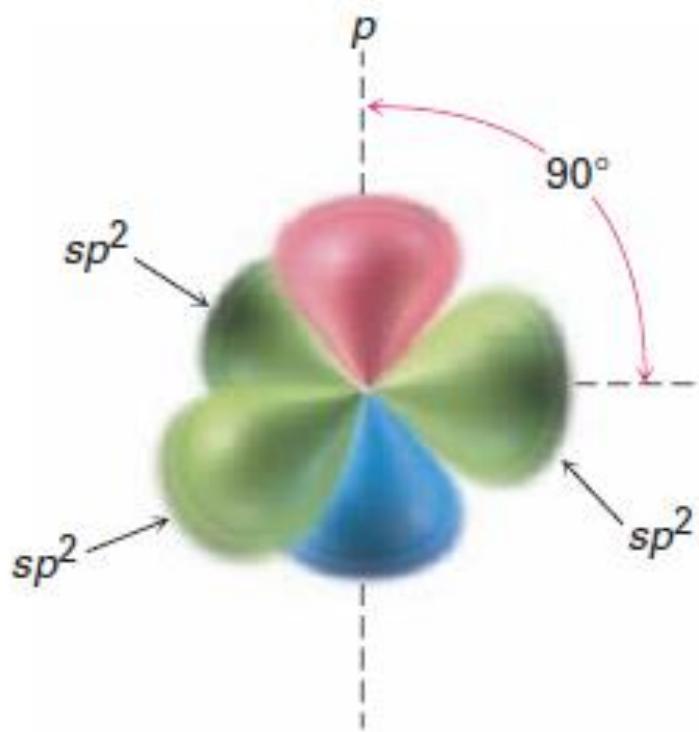


Hexane

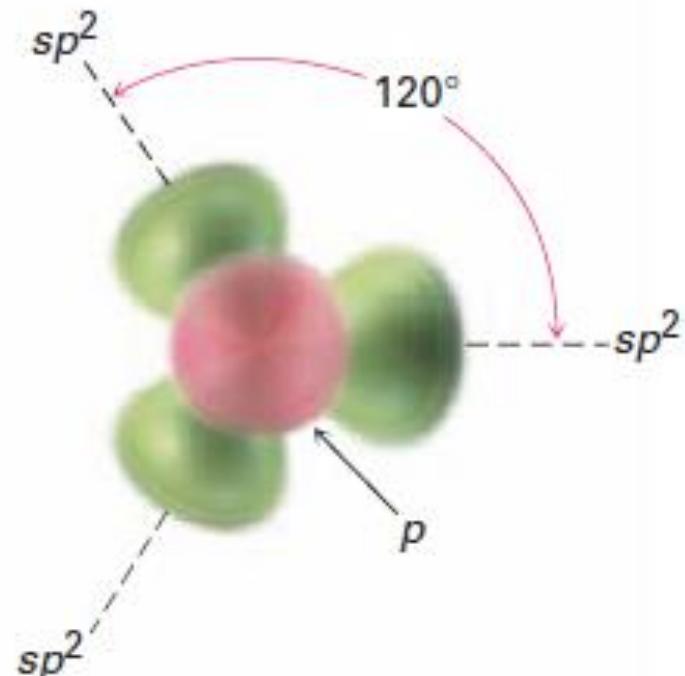


sp^2 hybridization

Lai hóa sp^2



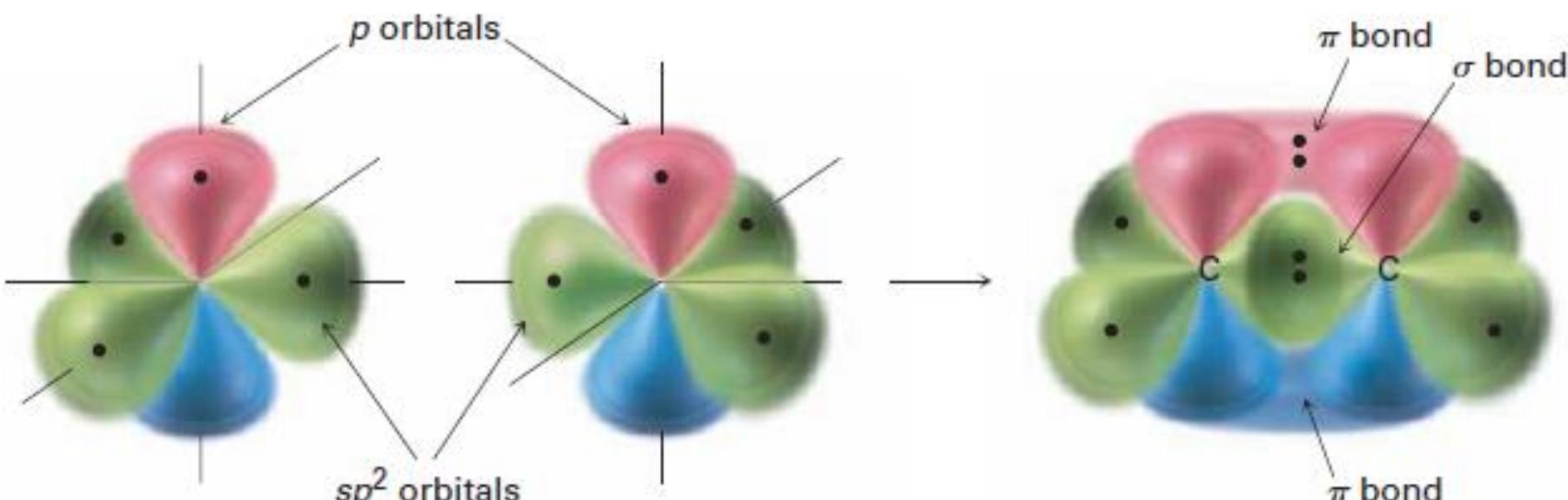
Side view



Top view



sp^2 hybridization: ethylene



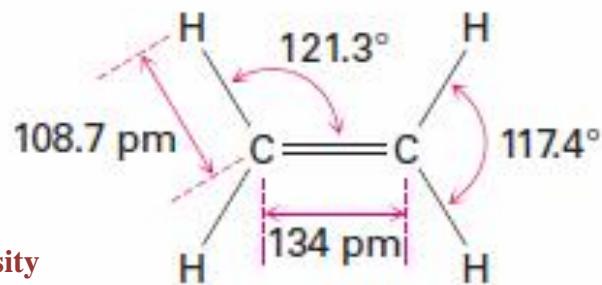
sp^2 carbon

sp^2 carbon

Carbon–carbon double bond

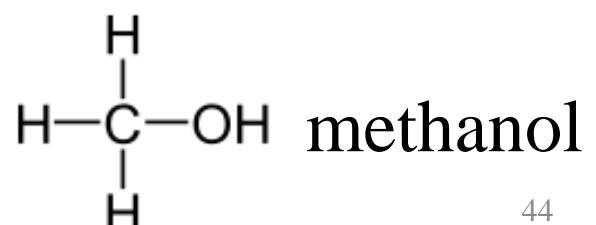
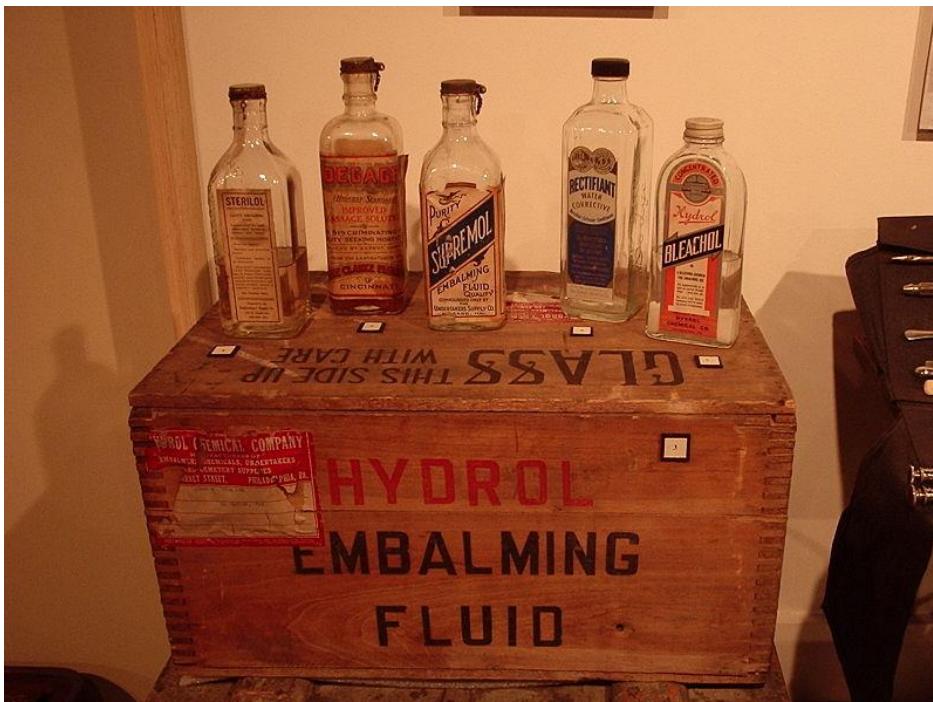


Lê Quốc Chơn - Duy Tân University



Problem

Draw electron-dot and line-bond structure of formaldehyde (HCHO) and indicate the hybridization of this substance?





Rosalia Lombardo 1918-1920 in Sicily, Italia

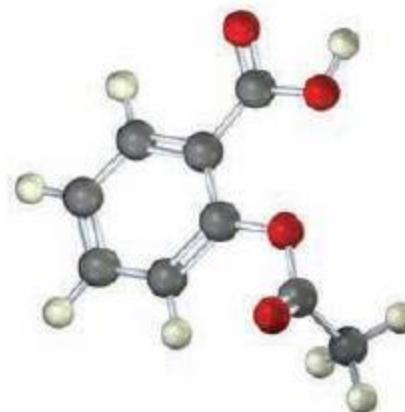


Problem 1.10-1.12

Draw line-bond structure of propene, 1,3- butadiene.
Indicate the hybridization of the orbitals on each carbon
and value of each bond angle.

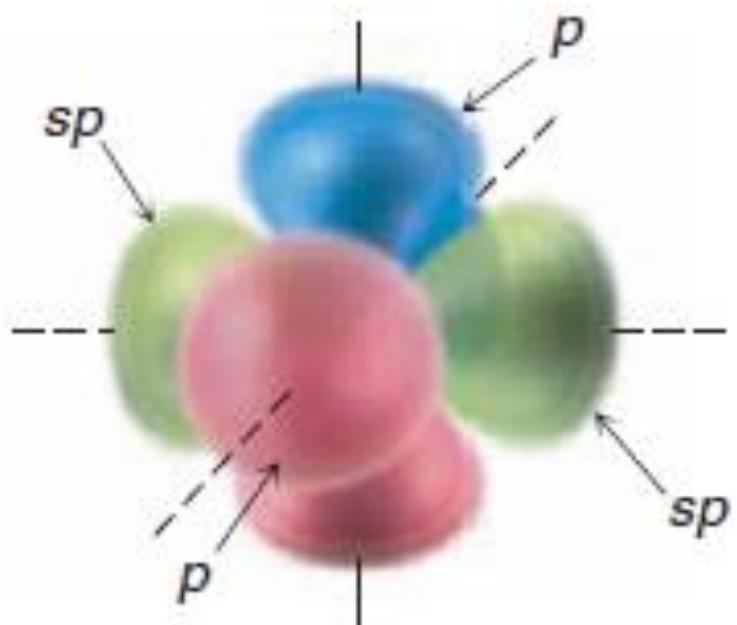
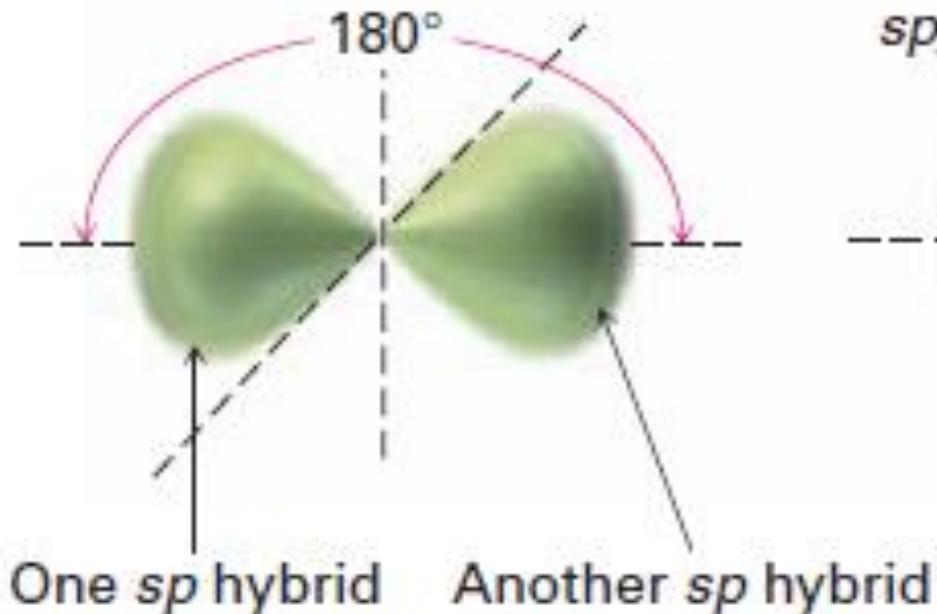
Look at structure of aspirin (acetylsalicylic acid)
and identify the orbital hybridization and tell
which atoms have lone pairs of electrons.

Red: oxygen
Grey: carbon
Ivory: hydrogen

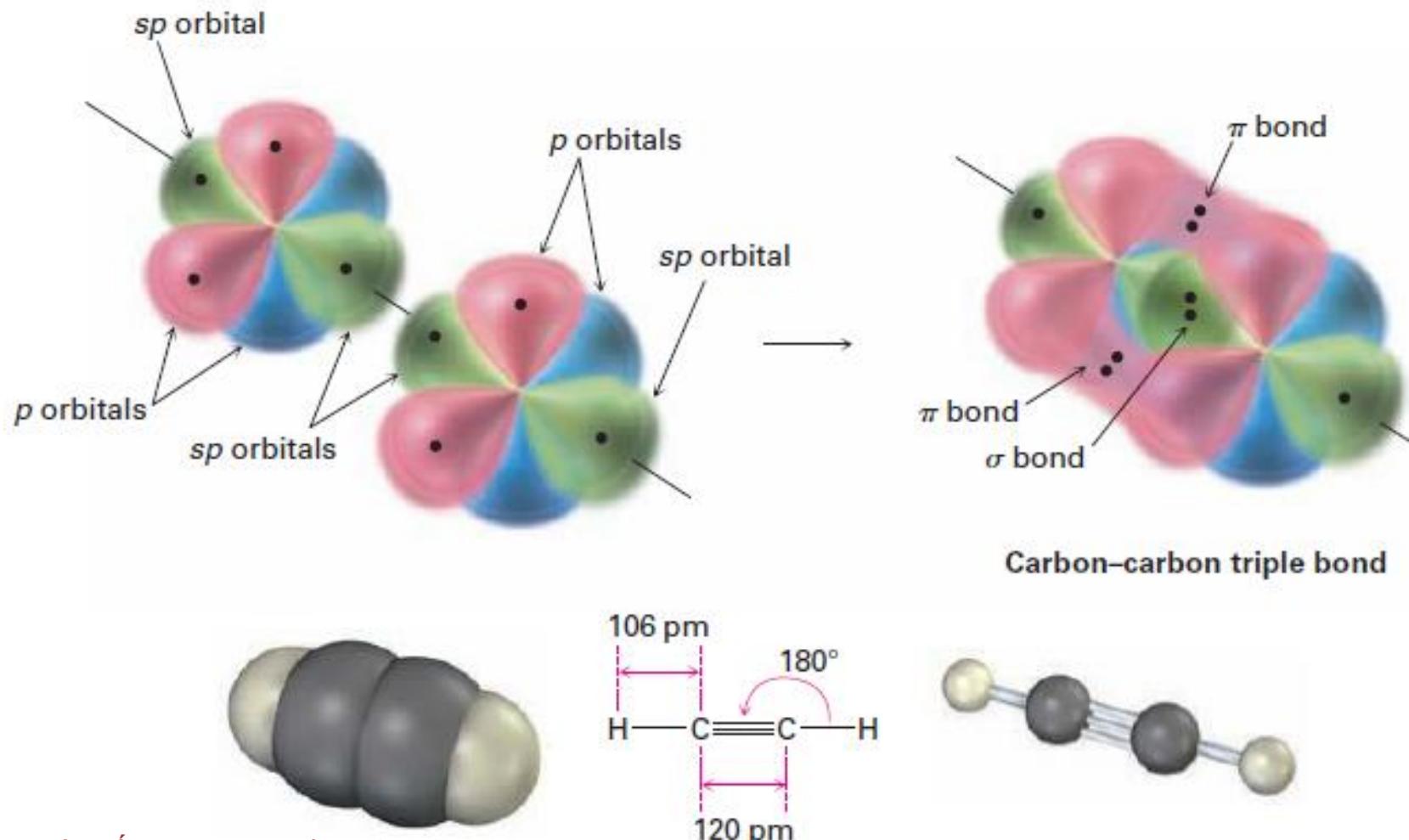


sp hybridization

Lai hóa sp



sp hybridization



Problem 1.13

Draw a line-bond structure for propyne, C₃H₄. Indicate the hybridization of the orbitals on each carbon, predict bond angle.



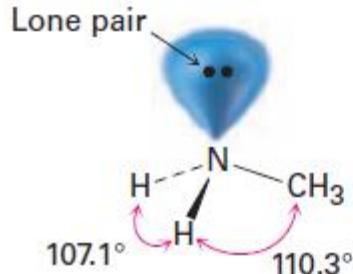
Summary

TABLE 1-2 Comparison of C–C and C–H Bonds in Methane, Ethane, Ethylene, and Acetylene

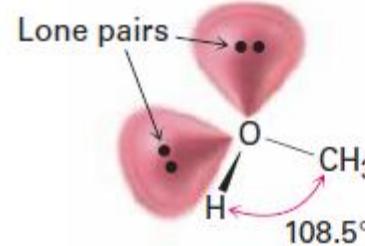
Molecule	Bond	Bond strength		Bond length (pm)
		(kJ/mol)	(kcal/mol)	
Methane, CH ₄	(sp ³) C—H	439	105	109
Ethane, CH ₃ CH ₃	(sp ³) C—C (sp ³)	377	90	154
	(sp ³) C—H	421	101	109
Ethylene, H ₂ C=CH ₂	(sp ²) C=C (sp ²)	728	174	134
	(sp ²) C—H	464	111	109
Acetylene, HC≡CH	(sp) C≡C (sp)	965	231	120
	(sp) C—H	558	133	106



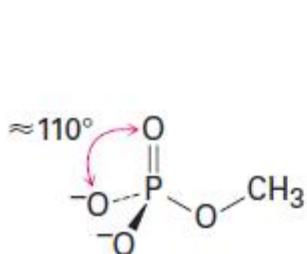
Hybridization of N, O, S



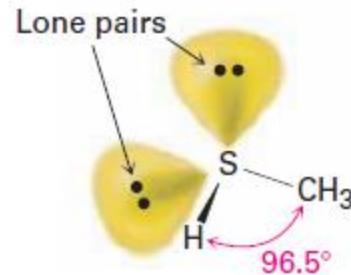
Methylamine



Methanol
(methyl alcohol)



Methyl phosphate
(an organophosphate)



Methanethiol

Orbital hybridization can also apply to N, O, S and P.

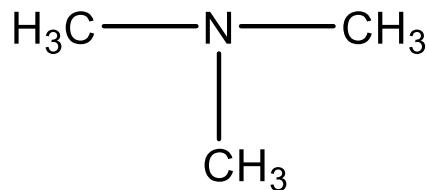


Problem 1.14

Identify the nonbonding lone pairs of electrons of atom O, N, P and S in the following molecules. Can you predict the angle between substituents attached to those atoms?



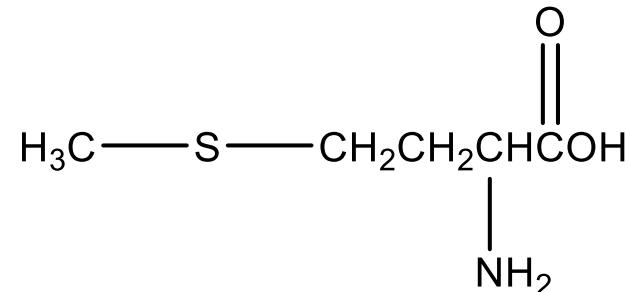
dimethyl ether



trimethylamine



phosphine



amino acid methionine



Molecular orbital theory

(Thuyết orbital phân tử)

Atomic orbitals versus molecular orbitals

Overlapping versus combination (additive or subtractive)



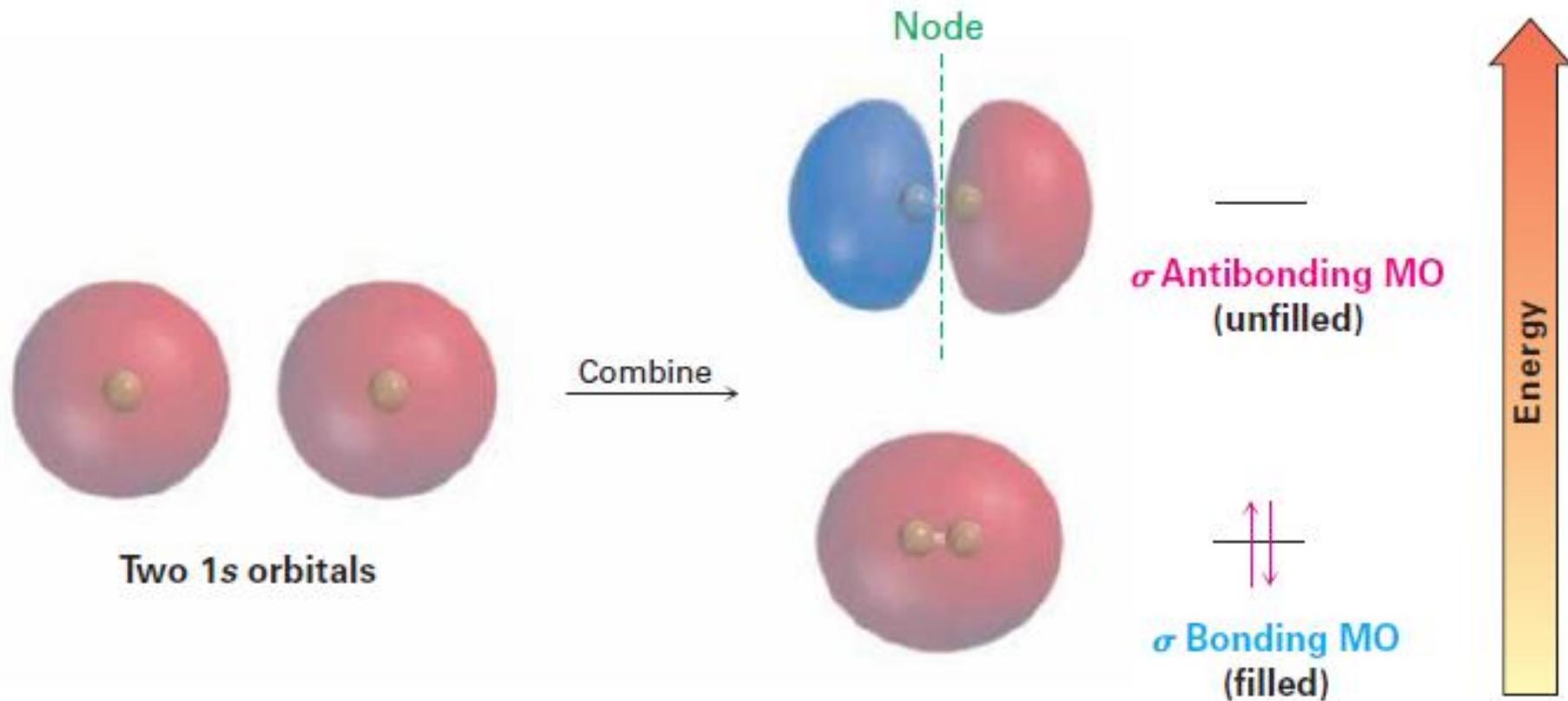
Overlapping or not



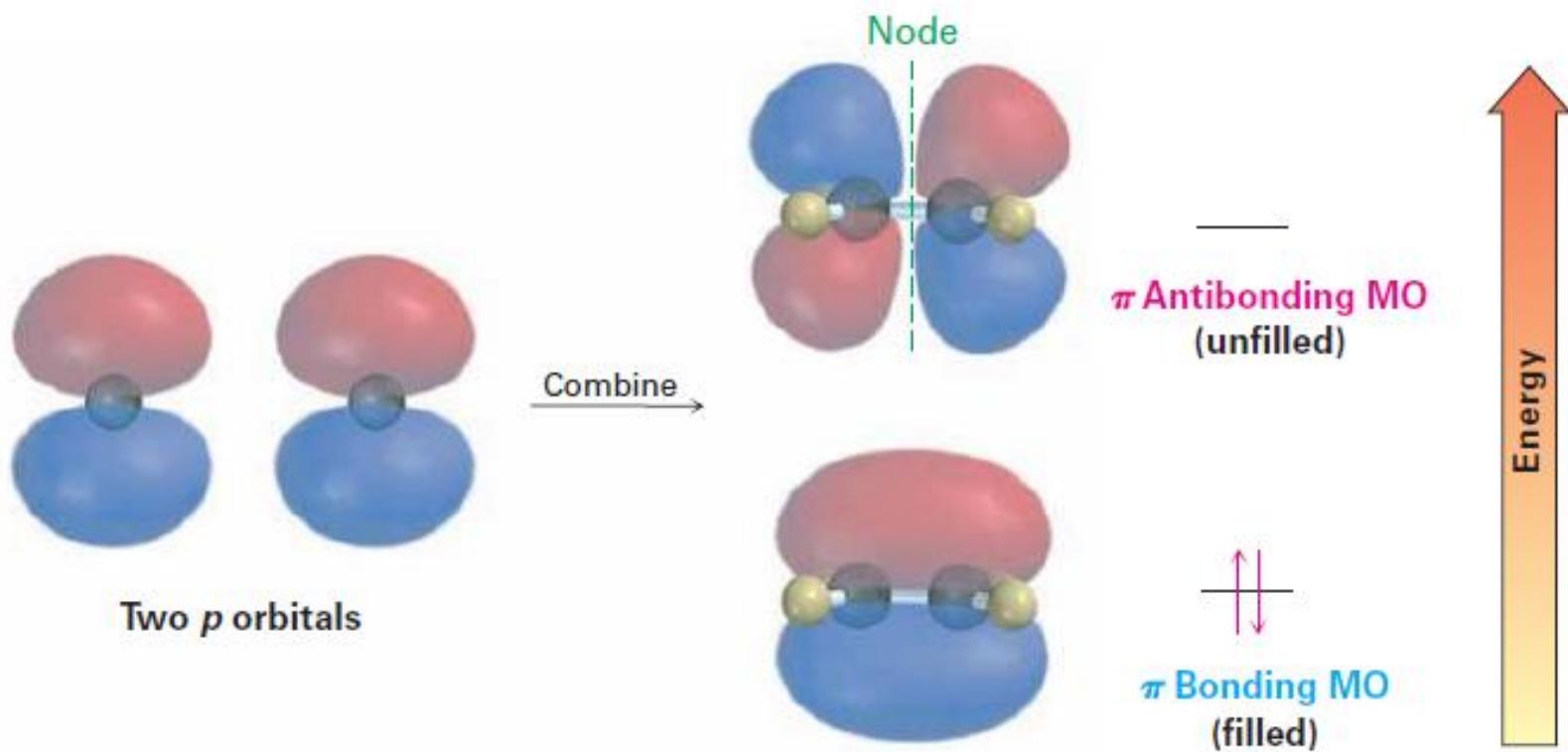
bonding MO or antibonding MO



Molecular orbital theory



Molecular orbital theory

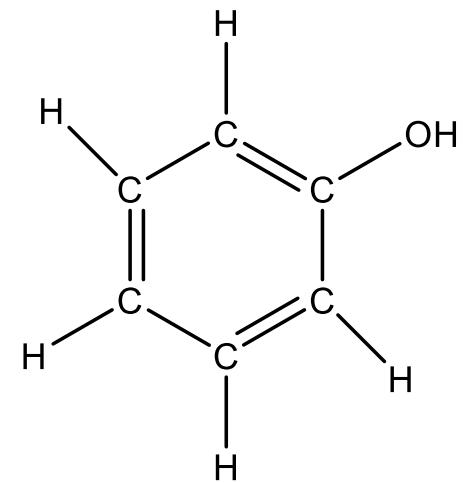


Drawing Chemical Structures

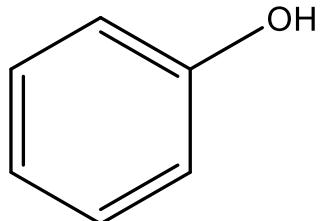
Condensed structures



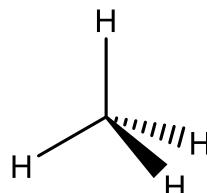
Kekulé structures



Skeletal structure



Wedged, dashed, line structures



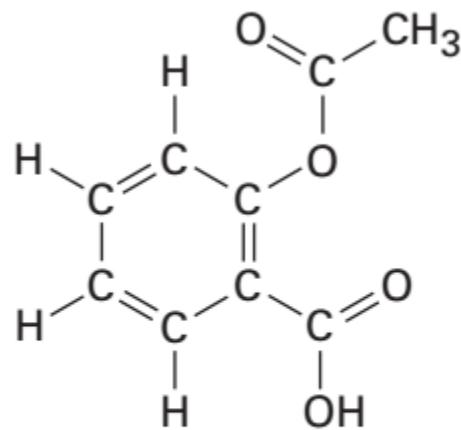
Problems

Are you ready with Paper and Pen?



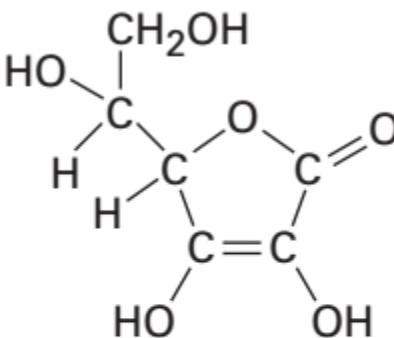
1. Convert the following line-bond structures into molecular formulas

(a)



Aspirin
(acetylsalicylic acid)

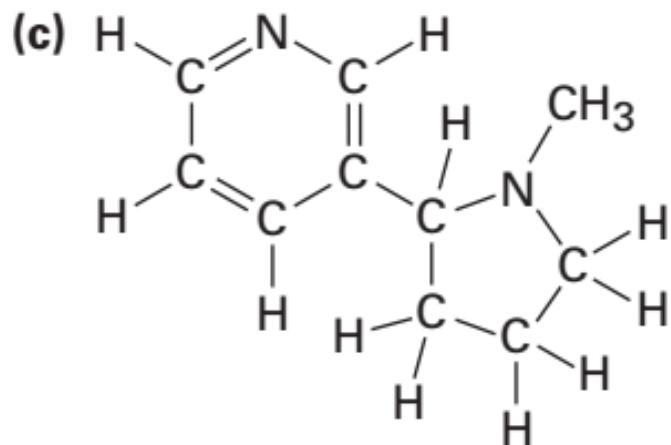
(b)



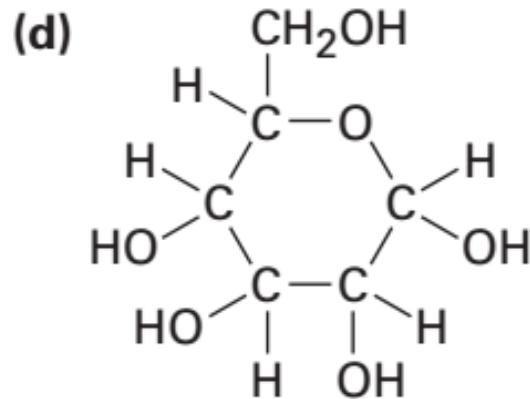
Vitamin C
(ascorbic acid)



2. Convert the following line-bond structures into molecular formulas



Nicotine



Glucose



3. Problem 1.17

Identify multiple bonds in this molecule and draw skeletal structure of it. Red = O, green = N, ivory = H



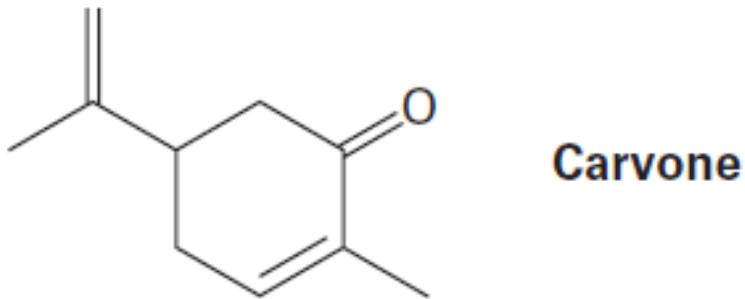
para-Aminobenzoic acid
(PABA)

(it was used as active ingredient in sunscreen to absorb UVB)



4. Problem

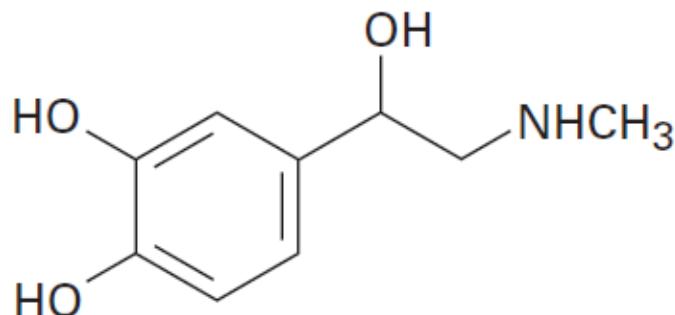
Give molecular formula of Carvone (odor of spearmint)



5. Problem 1.15

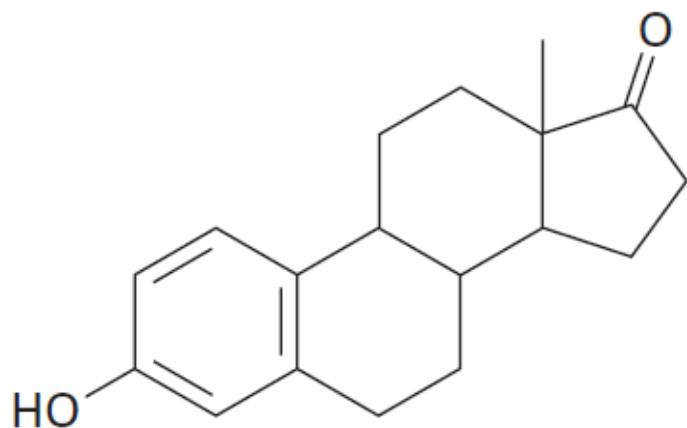
Give molecular formula of each substance:

(a)



Adrenaline

(b)



Estrone (a hormone)



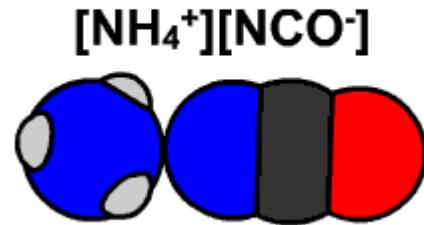
6. Problem 1.16

Propose skeletal structures for these following compounds (> 1 possibility):

- (a) C₅H₁₂ (b) C₂H₇N (c) C₃H₆O (d) C₄H₉Cl



Formation of Urea



Is there a crisis in organic chemistry education?

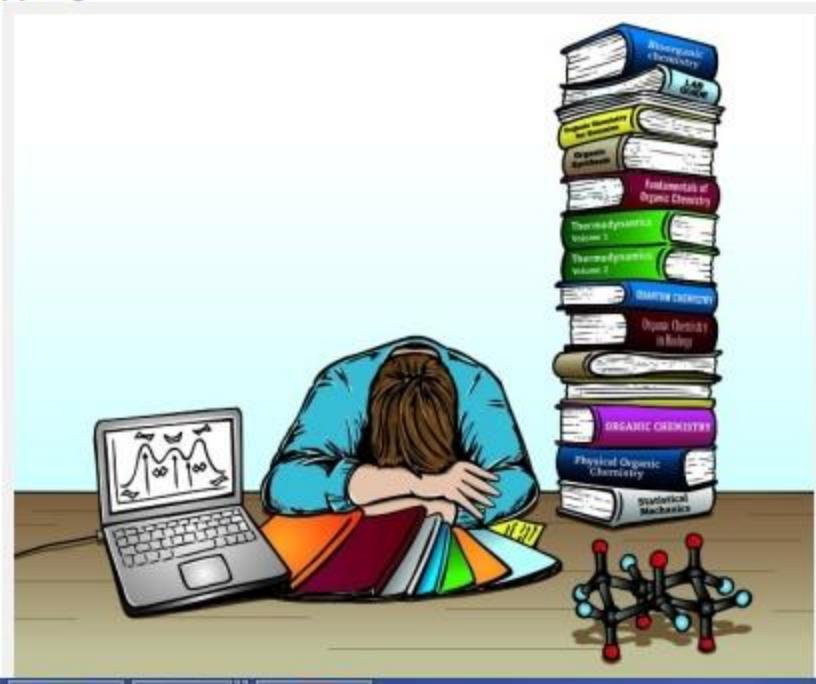
Teachers say yes, but most of the problems aren't new

By **Bethany Halford**

Symposium organizers drew attention to a session earlier this month at the ACS national meeting in San Diego with a provocative title: "Is There a Crisis in Organic Chemistry Education?" But many of the speakers—most of whom work in academic publishing—responded with a "no," threatening to deflate the advertised anxiety.

Quite the contrary, they said. Never before have organic chemistry students and teachers had so many resources at

[+]Enlarge





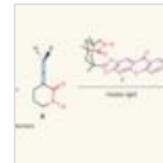
Organic chemistry

Atom RSS Feed

Organic chemistry is the study of **the synthesis, structure, reactivity and properties** of the diverse group of chemical compounds primarily constructed of carbon. All life on earth is carbon-based, thus organic chemistry is also the basis of biochemistry. The ability to form compounds containing long chains of carbon atoms is the basis of polymer chemistry.

News and Views | 12 December 2018

An exciting tool for asymmetric synthesis



<https://www.nature.com/subjects/organic-chemistry>

Cheng Yang & Yoshihisa Inoue

Nature **564**, 197–199

Related Subjects

Carbohydrate chemistry

Combinatorial libraries

Synthetic chemistry methodology

Microwave chemistry

Natural product synthesis

Reaction mechanisms

Stereochemistry

Structure elucidation

