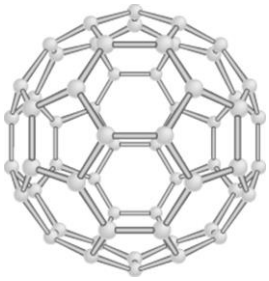
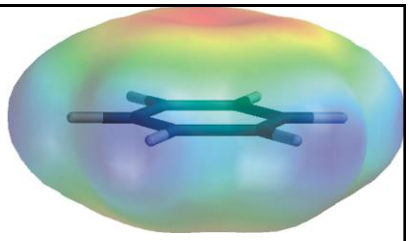




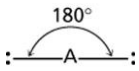
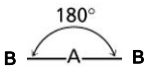
پیوند شیمیایی II:
شکل هندسی مولکول و هیبریداسیون اوربیتال های اتمی

فصل دهم

نظریه دافعه جفت الکترون ظرفیت (VSEPR)

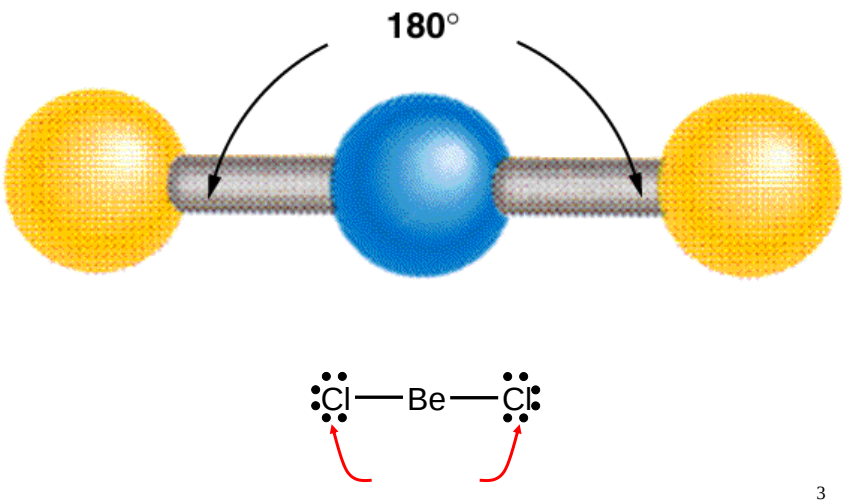
Valence shell electron pair repulsion

شکل هندسی مولکول ها را از دافعه الکتروستاتیکی بین جفت الکترون ها (پیوندی و ناپیوندی) پیش بینی می کند.

Class	تعداد اتم های پیوند شده به اتم مرکزی	تعداد جفت الکترون های ناپیوندی بر روی اتم مرکزی	نحوه قرار گرفتن جفت الکترون ها	شکل هندسی مولکول
AB_2	2	0		

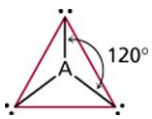
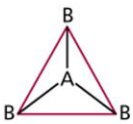
2

Beryllium Chloride



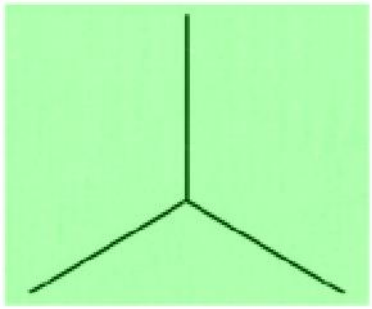
3

VSEPR

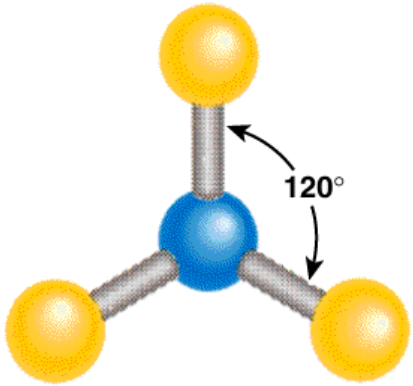
Class	تعداد اتم های پیوند شده به اتم مرکزی	تعداد جفت الکترون های ناپیوندی بر روی اتم مرکزی	نحوه قرار گرفتن جفت الکترون ها	شکل هندسی مولکول
AB_2	2	0	خطی	خطی
AB_3				

4

Boron Trifluoride



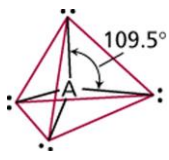
Planar

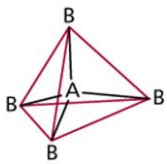


5

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_2	2	0	خطی	خطی
AB_3	3	0	مثلثی مسطح	مثلثی مسطح
AB_4				





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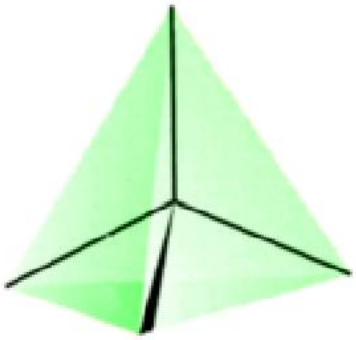
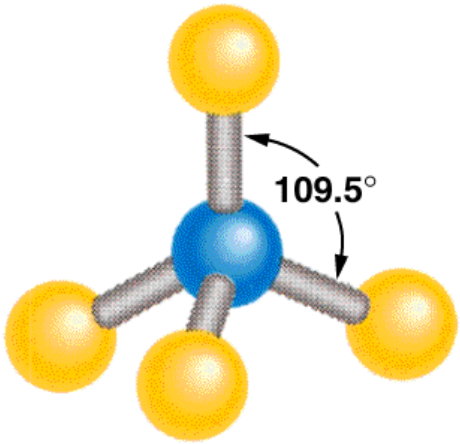
Methane



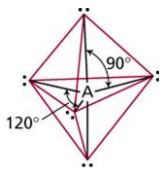
Tetrahedral

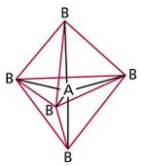


7

VSEPR

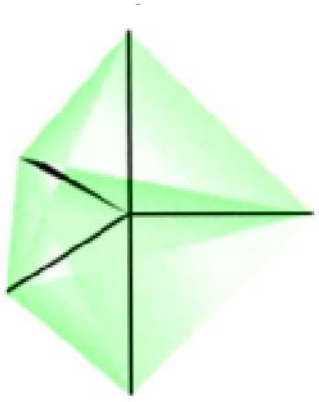
Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_2	2	0	خطی	خطی
AB_3	3	0	مثلثی مسطح	مثلثی مسطح
AB_4	4	0	چهار وجهی	چهار وجهی
AB_5				



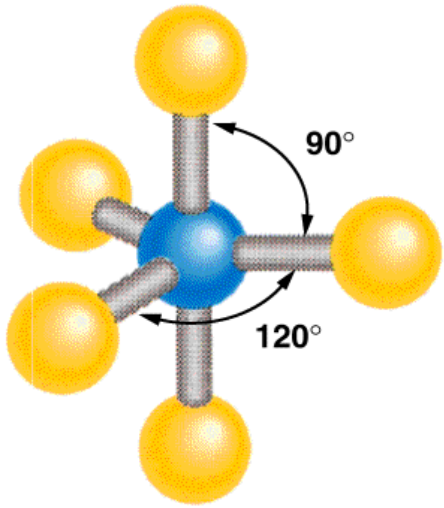


8

Phosphorus Pentachloride

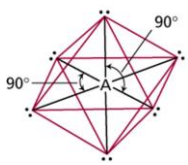
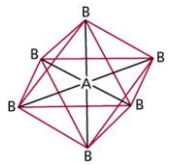


Trigonal bipyramidal

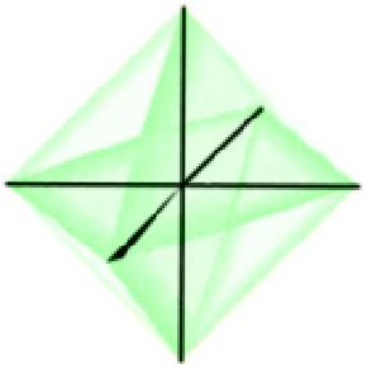


9

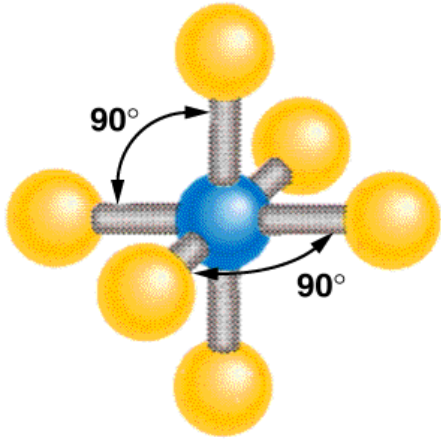
VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_2	2	0	خطی	خطی
AB_3	3	0	مثلثی مسطح	مثلثی مسطح
AB_4	4	0	چهار وجهی	چهار وجهی
AB_5	5	0	دو هرمی مثلثی	دو هرمی مثلثی
AB_6				

Sulfur Hexafluoride



Octahedral



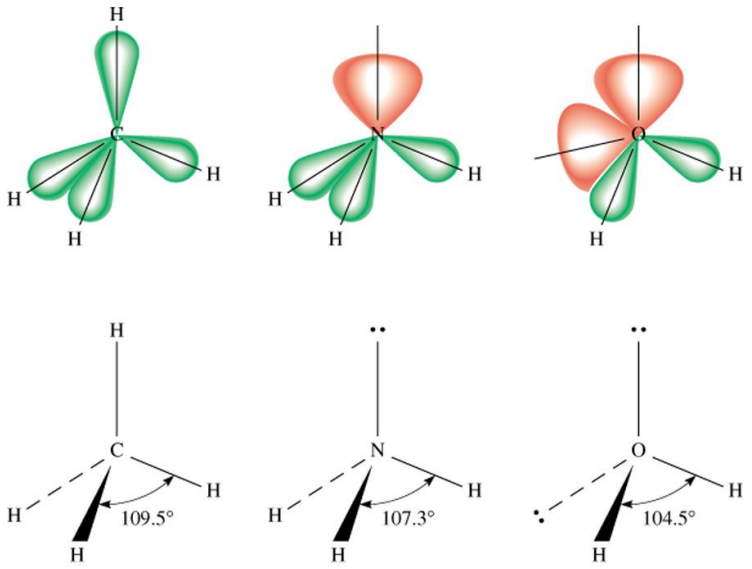
11

TABLE 10.1 Arrangement of Electron Pairs About a Central Atom (A) in a Molecule and Geometry of Some Simple Molecules and Ions in Which the Central Atom Has No Lone Pairs

Number of Electron Pairs	Arrangement of Electron Pairs*	Molecular Geometry*	Examples
2	180° Linear	B—A—B Linear	$BeCl_2$, $HgCl_2$
3	120° Trigonal planar	Trigonal planar	BF_3
4	109.5° Tetrahedral	Tetrahedral	CH_4, NH_4^+
5	90°, 120° Trigonal bipyramidal	Trigonal bipyramidal	PCl_5
6	90°, 90° Octahedral	Octahedral	SF_6

*The colored lines are used only to show the overall shapes; they do not represent bonds.

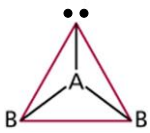
12

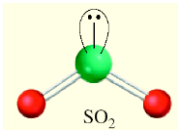


13

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_3	3	0	مثلثی مسطح	مثلثی مسطح
AB_2E				

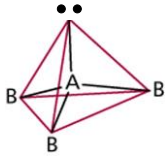


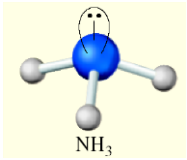


14

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_4	4	0	چهاروجهی	چهاروجهی
AB_3E				

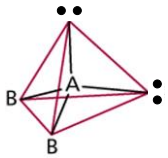


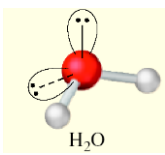


15

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_4	4	0	چهاروجهی	چهاروجهی
AB_3E	3	1	چهاروجهی	هرمی مثلثی
AB_2E_2				

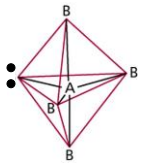


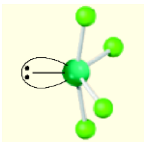


16

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_5	5	0	دوهرمی مثلثی	دوهرمی مثلثی
AB_4E				

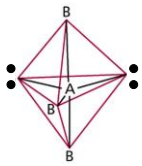


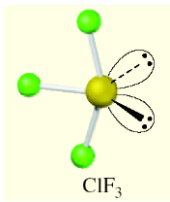


17

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_5	5	0	دوهرمی مثلثی	دوهرمی مثلثی
AB_4E	4	1	دوهرمی مثلثی	چهاروجهی نامنظم
AB_3E_2				

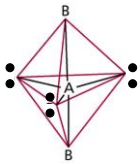


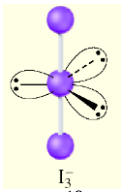


18

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_5	5	0	دوهرمی مثلثی	دوهرمی مثلثی
AB_4E	4	1	دوهرمی مثلثی	چهاروجهی نامنظم
AB_3E_2	3	2	دوهرمی مثلثی	T–شکل
AB_2E_3				





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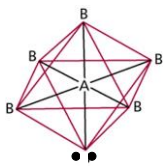
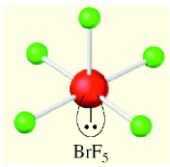
VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_6	6	0	هشت وجهی	هشت وجهی
AB_5E				

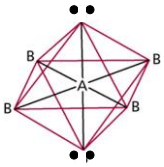




20

VSEPR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Arrangement of electron pairs	Molecular Geometry
AB_6	6	0	هشت وجهی	هشت وجهی
AB_5E	5	1	هشت وجهی	هرم مربع القاعده
AB_4E_2				



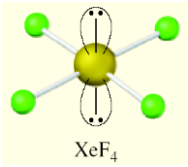


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TABLE 10.2 Geometry of Simple Molecules and Ions in Which the Central Atom Has One or More Lone Pairs

Class of Molecule	Total Number of Electron Pairs	Number of Bonding Pairs	Number of Lone Pairs	Arrangement of Electron Pairs*	Geometry of Molecule or Ion	Examples
AB_2E	3	2	1	Trigonal planar	Bent	SO_2
AB_3E	4	3	1	Tetrahedral	Trigonal pyramidal	NH_3
AB_2E_2	4	2	2	Tetrahedral	Bent	H_2O
AB_4E	5	4	1	Trigonal bipyramidal	Distorted tetrahedron (or seesaw)	SF_4
AB_3E_2	5	3	2	Trigonal bipyramidal	T-shaped	ClF_3
AB_2E_3	5	2	3	Trigonal bipyramidal	Linear	I_3^-
AB_5E	6	5	1	Octahedral	Square pyramidal	BrF_5
AB_4E_2	6	4	2	Octahedral	Square planar	XeF_4

*The colored lines are used to show the overall shape, not bonds.

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پیش بینی شکل هندسی مولکول

1. ساختار لوئیس را رسم کنید.
2. تعداد جفت الکترون های روی اتم مرکزی و تعداد اتم های متصل شده به اتم مرکزی را بشمارید.
3. از VSEPR استفاده کنید و شکل هندسی مولکول را پیش بینی کنید.

What are the molecular geometries of SO_2 and SF_4?

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Section 8.13

Molecular Structure: The VSEPR Model

Determine the shape for each of the following molecules, and include bond angles:

HCN

PH_3

SF_4

Return to TOC

24

Section 8.13

Molecular Structure: The VSEPR Model

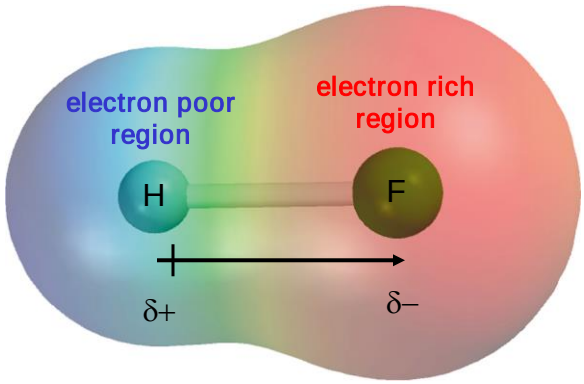
Determine the shape for each of the following molecules, and include bond angles:

O_3

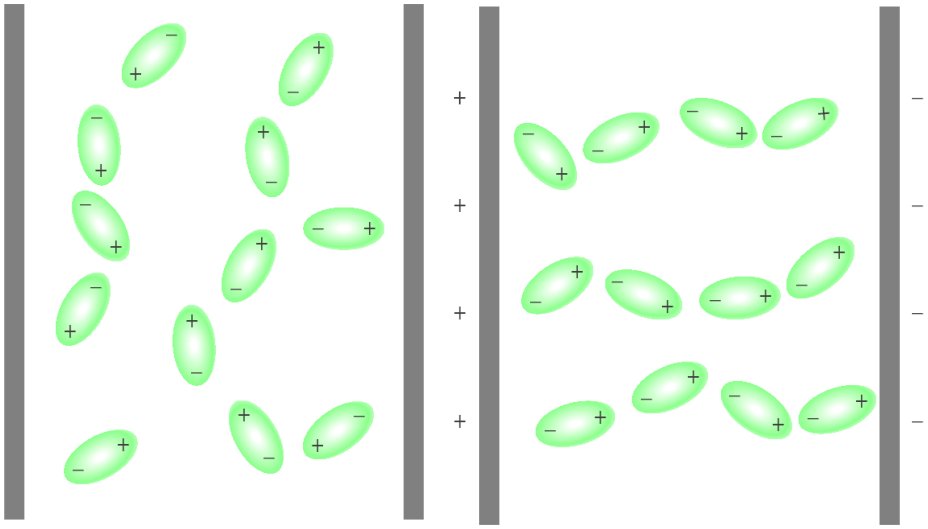
KrF_4

Return to TOC

ممان دو قطبی و مولکول های قطبی



رفتار مولکول های قطبی



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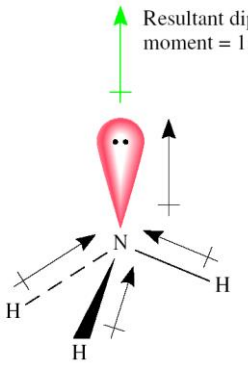
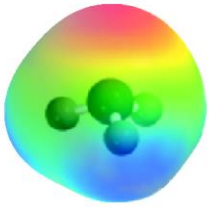
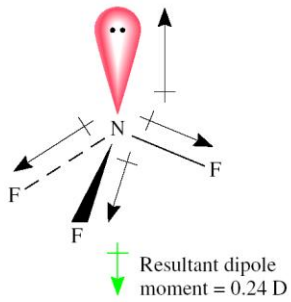
27

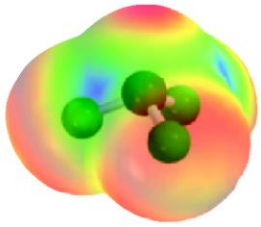
پیوندهای قطبی و حاصل ممان های دو قطبی در NH_3 و NF_3







Resultant dipole
moment = 0.24 D



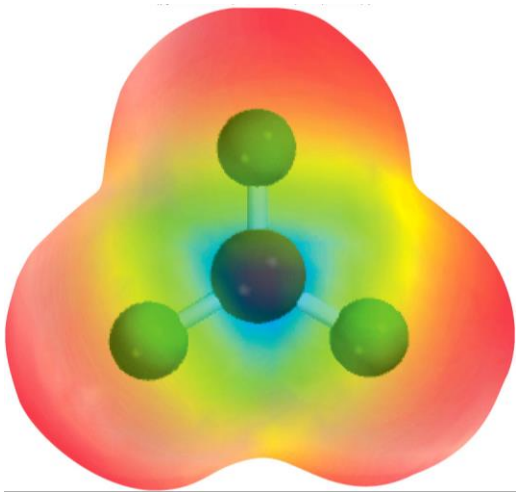
28

کدامیک از مولکول های زیر ممان دو قطبی دارد؟

H_2O, CO_2, SO_2, and CF_4

29

Does BF_3 have a dipole moment?



30

Does CH_2Cl_2 have a dipole moment?

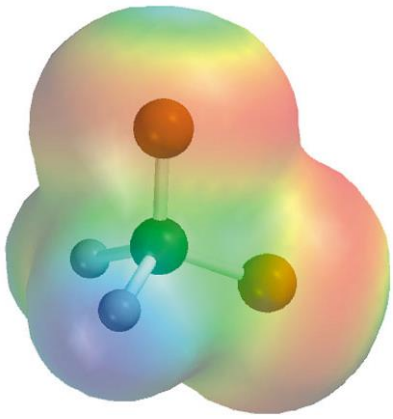


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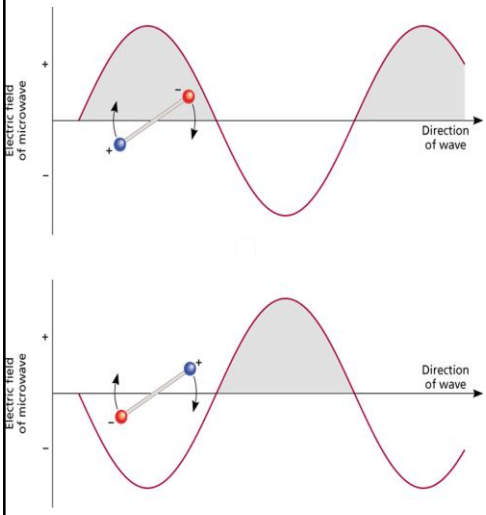
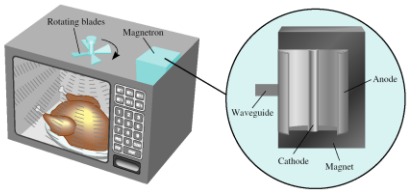
TABLE 10.3 Dipole Moments of Some Polar Molecules

Molecule	Geometry	Dipole Moment (D)
HF	Linear	1.92
HCl	Linear	1.08
HBr	Linear	0.78
HI	Linear	0.38
H_2O	Bent	1.87
H_2S	Bent	1.10
NH_3	Trigonal pyramidal	1.46
SO_2	Bent	1.60

32

Chemistry In Action: Microwave Ovens





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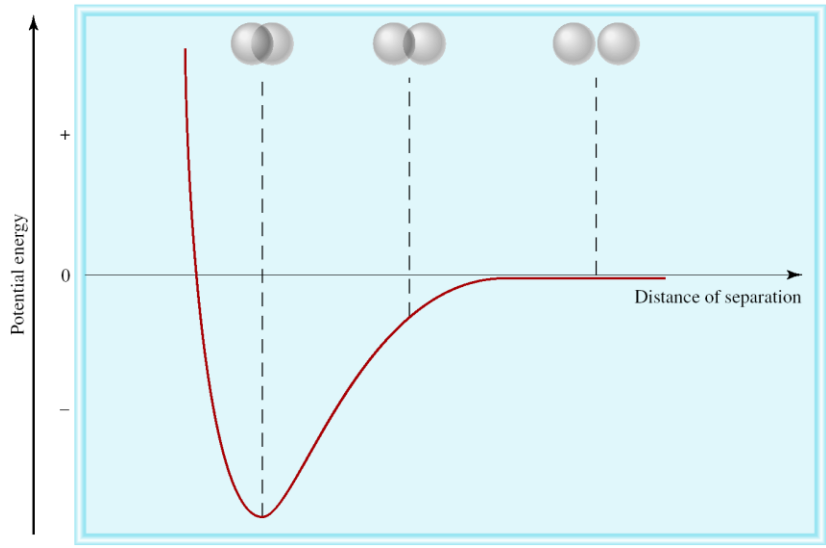
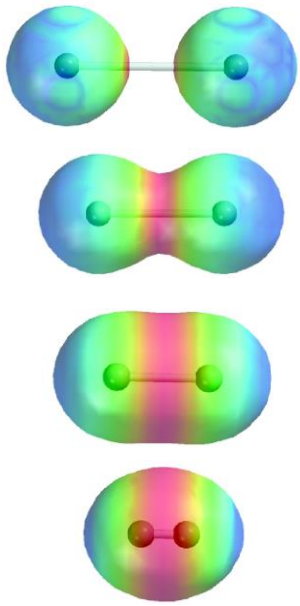
	Bond Enthalpy	Bond Length	Overlap Of
H_2	436.4 kJ/mol	74 pm	2 1*s*
F_2	150.6 kJ/mol	142 pm	2 2*p*

34



35



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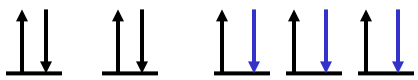
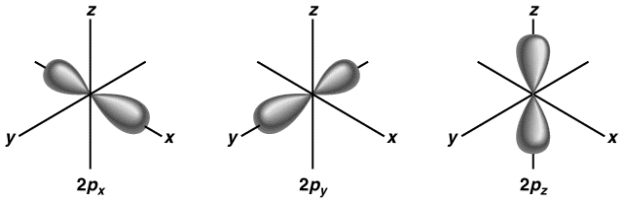
Valence Bond Theory and NH_3

N – $1s^2 2s^2 2p^3$

3 H – $1s^1$





If use the 3 2*p* orbitals predict 90°

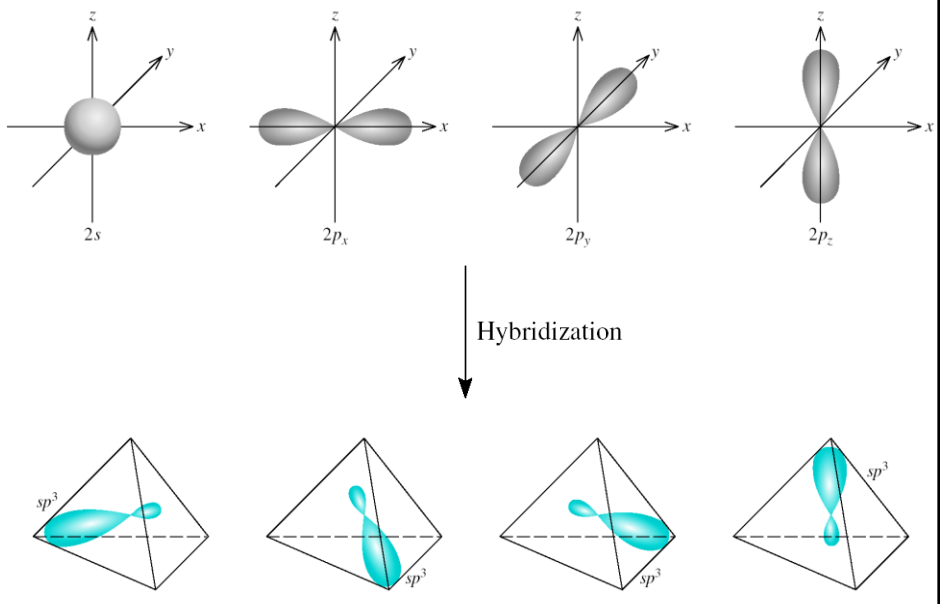
Actual H-N-H bond angle is 107.3°

37

Hybridization – mixing of two or more atomic orbitals to form a new set of hybrid orbitals.

38

Formation of sp^3 Hybrid Orbitals



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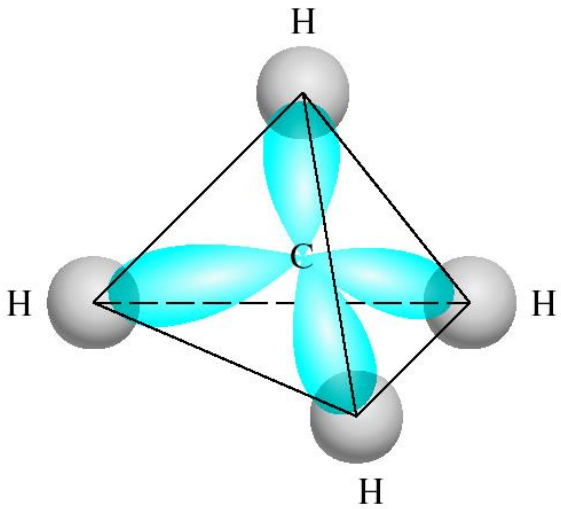
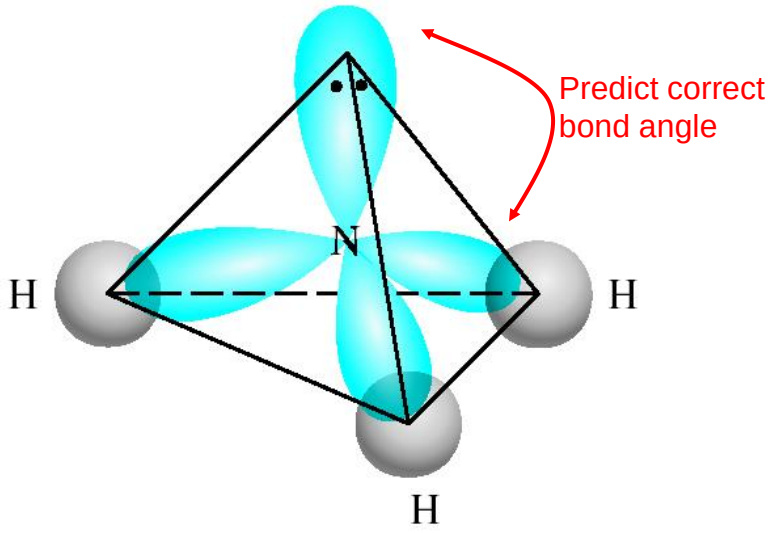
Formation of Covalent Bonds in CH_4



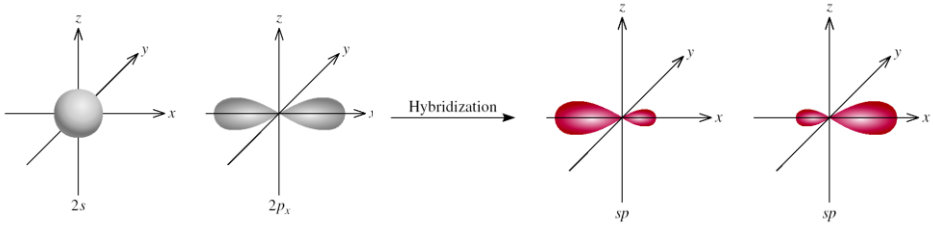
40

sp^3-Hybridized N Atom in NH_3



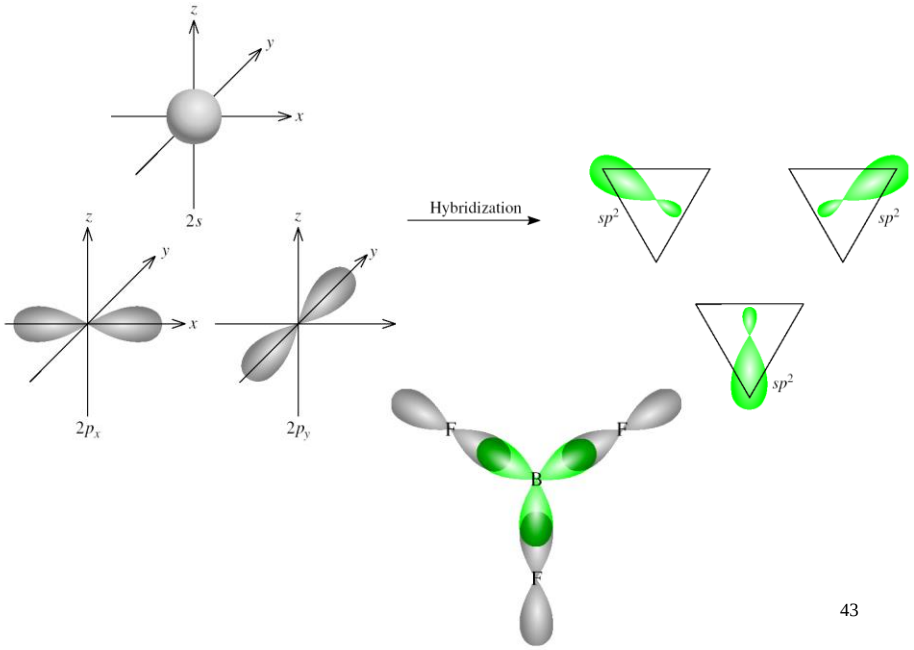
41

Formation of *sp* Hybrid Orbitals



42

Formation of sp^2 Hybrid Orbitals



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How do I predict the hybridization of the central atom?

1. Draw the Lewis structure of the molecule.
2. Count the number of lone pairs AND the number of atoms bonded to the central atom

# of Lone Pairs + # of Bonded Atoms	Hybridization	Examples
2	sp	$BeCl_2$
3	sp^2	BF_3
4	sp^3	CH_4, NH_3, H_2O
5	sp^3d	PCl_5
6	sp^3d^2	SF_6

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TABLE 10.4 Important Hybrid Orbitals and Their Shapes

Pure Atomic Orbitals of the Central Atom	Hybridization of the Central Atom	Number of Hybrid Orbitals	Shape of Hybrid Orbitals	Examples
s, *p*	*sp*	2	180° Linear	$BeCl_2$
s, *p*, *p*	sp^2	3	120° Trigonal planar	BF_3
s, *p*, *p*, *p*	sp^3	4	109.5° Tetrahedral	CH_4, NH_4^+
s, *p*, *p*, *p*, *d*	sp^3d	5	90°, 120° Trigonal bipyramidal	PCl_5
s, *p*, *p*, *p*, *d*, *d*	sp^3d^2	6	90°, 90° Octahedral	SF_6

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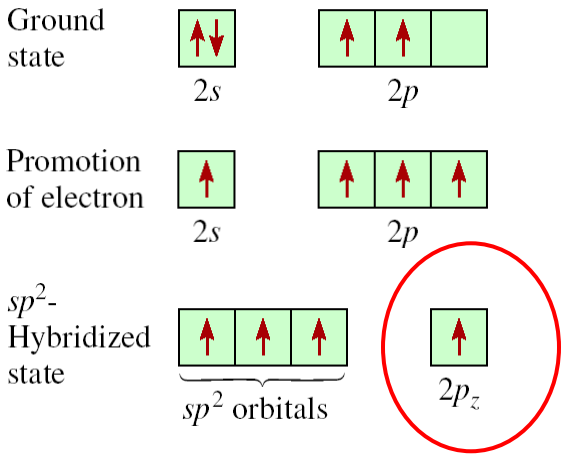
sp^2 Hybridization of Carbon



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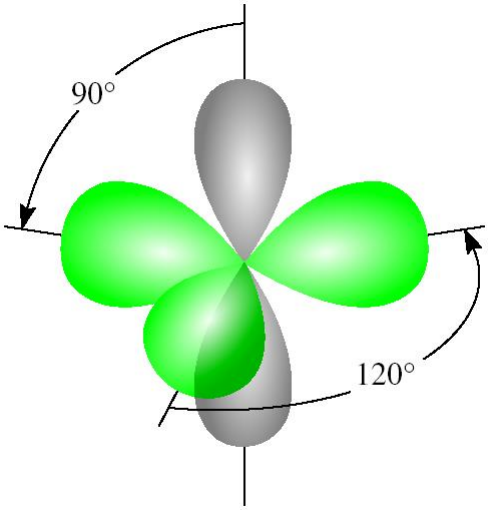
Unhybridized $2p_z$ orbital (gray), which is perpendicular to the plane of the hybrid (green) orbitals.



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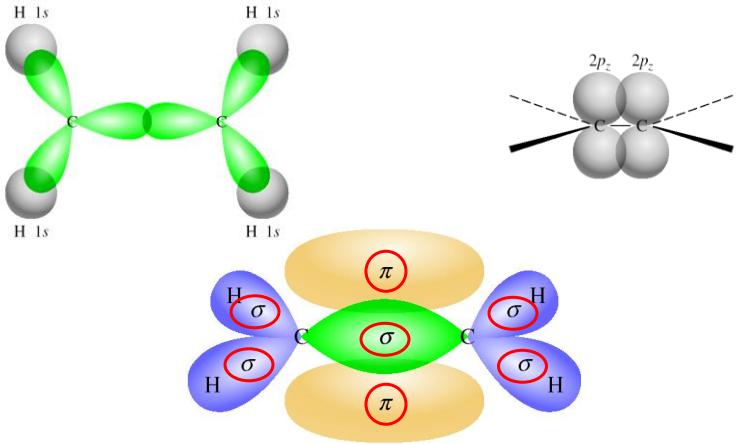
Bonding in Ethylene, C_2H_4

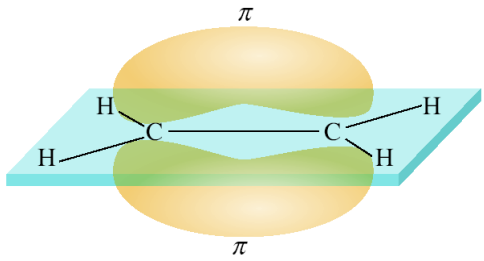


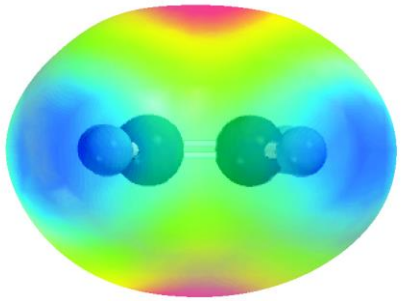
Sigma bond (σ) – electron density between the 2 atoms

Pi bond (π) – electron density above and below plane of nuclei of the bonding atoms

48

Another View of π Bonding in Ethylene, C_2H_4





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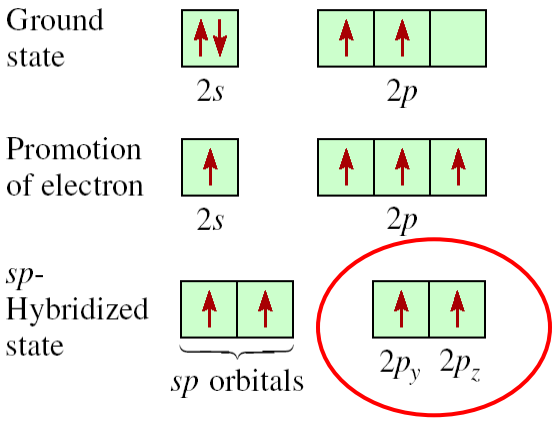
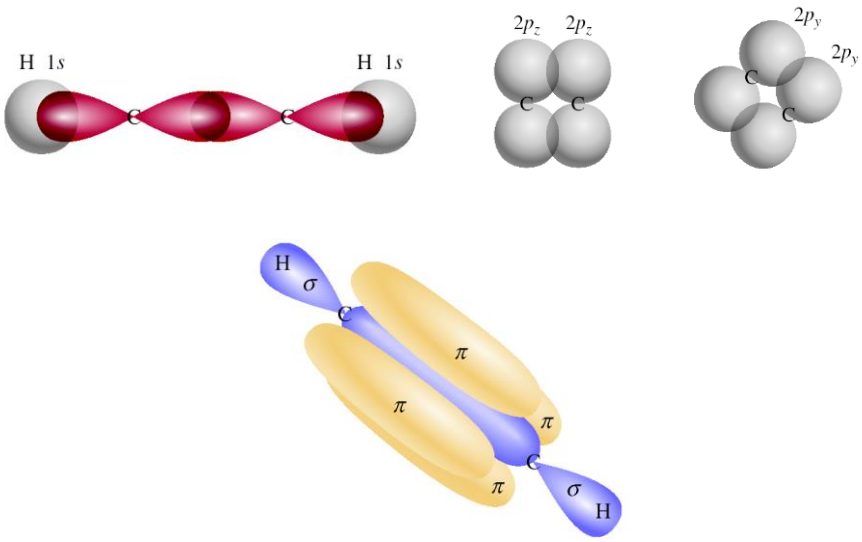
sp Hybridization of Carbon



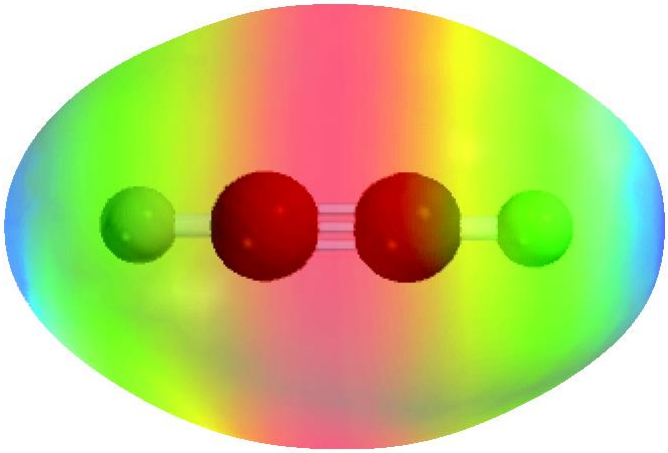
50

Bonding in Acetylene, C_2H_2



51

Another View of the Bonding in Ethylene, C_2H_4



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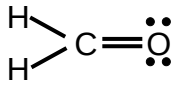
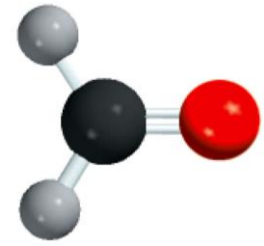
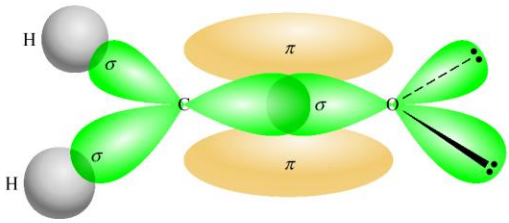
Describe the bonding in CH_2O.





CH_2O

C – 3 bonded atoms, 0 lone pairs
C – sp^2



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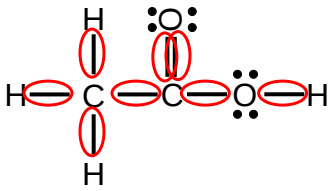
Sigma (σ) and Pi Bonds (π)

Single bond	1 sigma bond
Double bond	1 sigma bond and 1 pi bond
Triple bond	1 sigma bond and 2 pi bonds

How many σ and π bonds are in the acetic acid (vinegar) molecule CH_3COOH?



σ bonds = 6 + 1 = 7

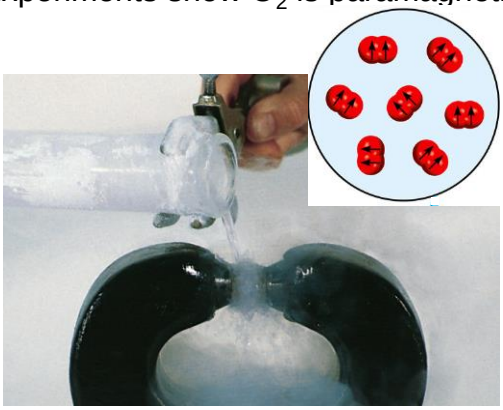
π bonds = 1

54

Experiments show O_2 is paramagnetic

No unpaired e^-

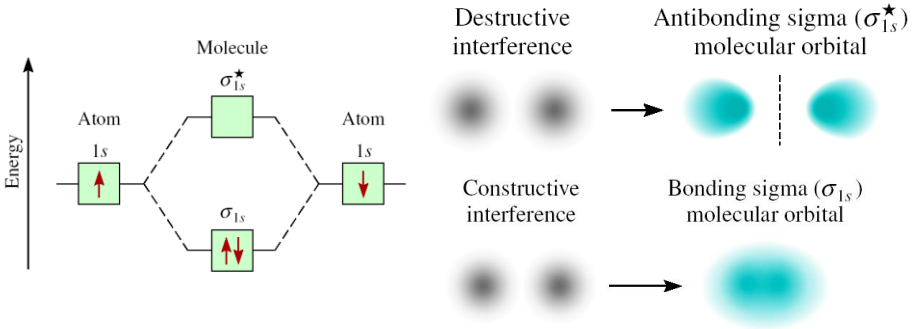
Should be diamagnetic



Molecular orbital theory – bonds are formed from interaction of atomic orbitals to form **molecular** orbitals.

55

Energy levels of bonding and antibonding **molecular** orbitals in hydrogen (H_2).



A ***bonding molecular orbital*** has lower energy and greater stability than the atomic orbitals from which it was formed.

An ***antibonding molecular orbital*** has higher energy and lower stability than the atomic orbitals from which it was formed.

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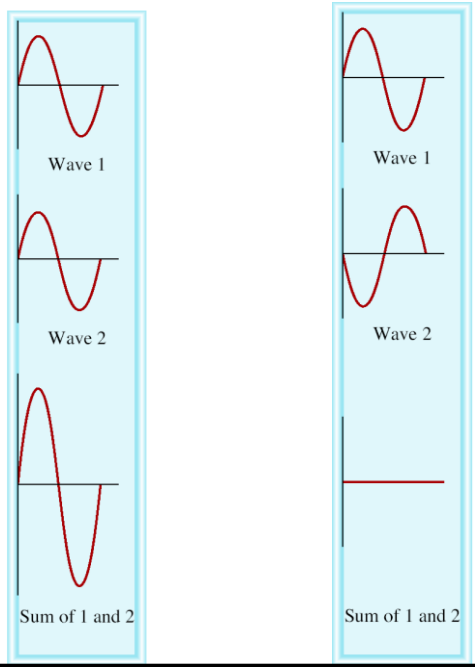
Constructive and Destructive Interference



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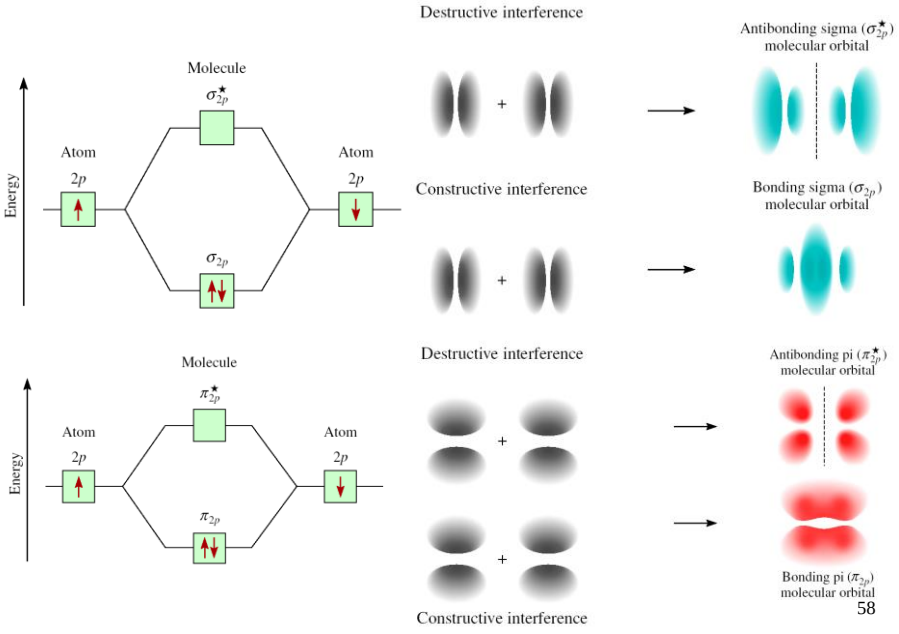
Two Possible Interactions Between Two Equivalent *p* Orbitals



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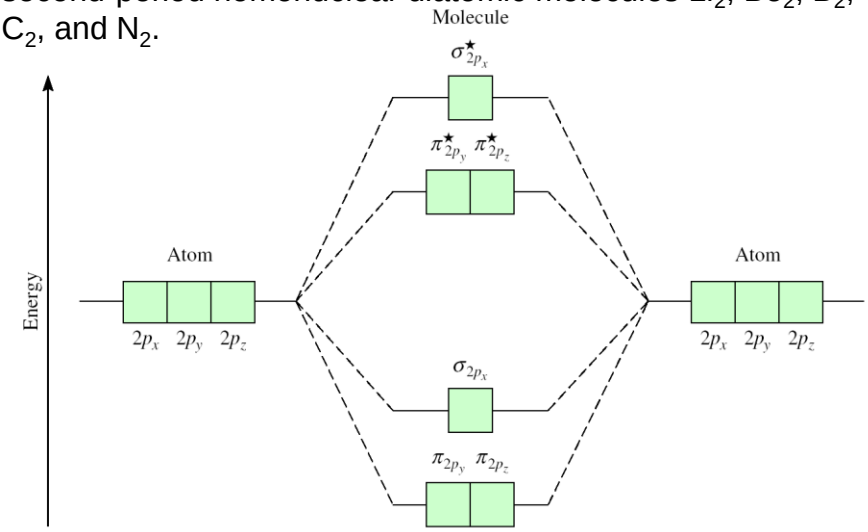
General molecular orbital energy level diagram for the second-period homonuclear diatomic molecules Li_2, Be_2, B_2, C_2, and N_2.



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Molecular Orbital (MO) Configurations

1. The number of molecular orbitals (MOs) formed is always equal to the number of atomic orbitals combined.
2. The more stable the bonding MO, the less stable the corresponding antibonding MO.
3. The filling of MOs proceeds from low to high energies.
4. Each MO can accommodate up to two electrons.
5. *Use Hund's rule when adding electrons to MOs of the* same energy.
6. The number of electrons in the MOs is equal to the sum of all the electrons on the bonding atoms.

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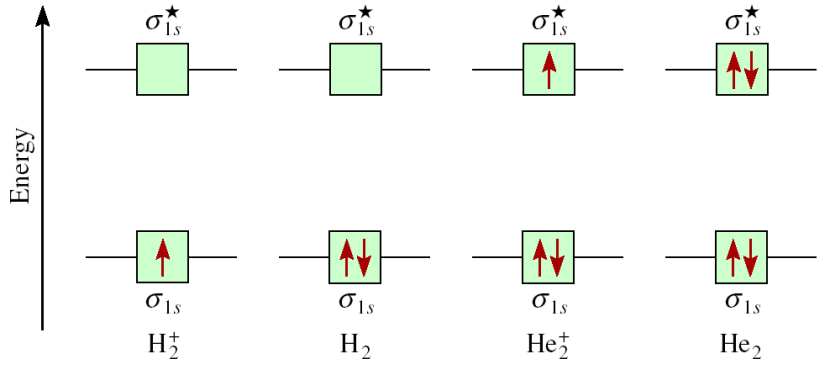
$$\text{bond order} = \frac{1}{2}\left(\text{Number of electrons in bonding MOs} - \text{Number of electrons in antibonding MOs}\right)$$



	H_2^+	H_2	He_2^+	He_2
bond order	½	1	½	0

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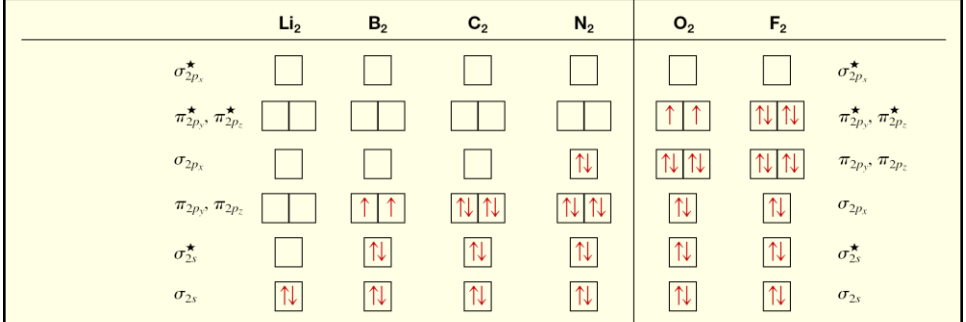
TABLE 10.5 Properties of Homonuclear Diatomic Molecules of the Second-Period Elements*



	Li_2	B_2	C_2	N_2	O_2	F_2
Bond order	1	1	2	3	2	1
Bond length (pm)	267	159	131	110	121	142
Bond enthalpy (kJ/mol)	104.6	288.7	627.6	941.4	498.7	156.9
Magnetic properties	Diamagnetic	Paramagnetic	Diamagnetic	Diamagnetic	Paramagnetic	Diamagnetic

*For simplicity the σ_{1s} and $\sigma^{\star}_{1s}$ orbitals are omitted. These two orbitals hold a total of four electrons. Remember that for O_2 and F_2, σ_{2p_x} is lower in energy than π_{2p_y} and π_{2p_z}.

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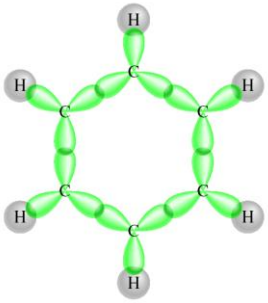
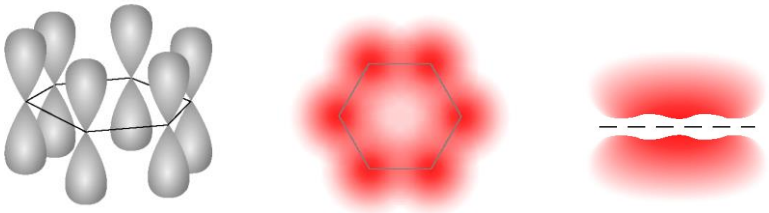
Delocalized molecular orbitals are not confined between two adjacent bonding atoms, but actually extend over three or more atoms.

Example: Benzene, C_6H_6



Delocalized π orbitals



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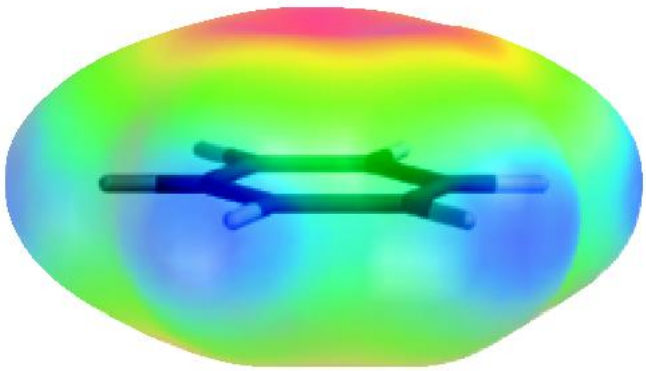
Electron density above and below the plane of the benzene molecule.



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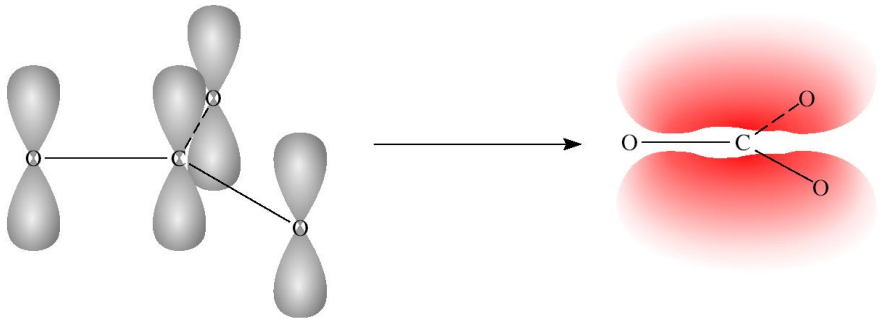
Bonding in the Carbonate Ion, CO_3^{2-}



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Chemistry In Action: Buckyball Anyone?