Molecules from Atoms

Lewis Dot Structures: Every valence electron illustrated by a dot.

Octet Rule: Atoms share (by *covalent* bonding), donate or accept electrons to achieve a filled outer shell of electrons.

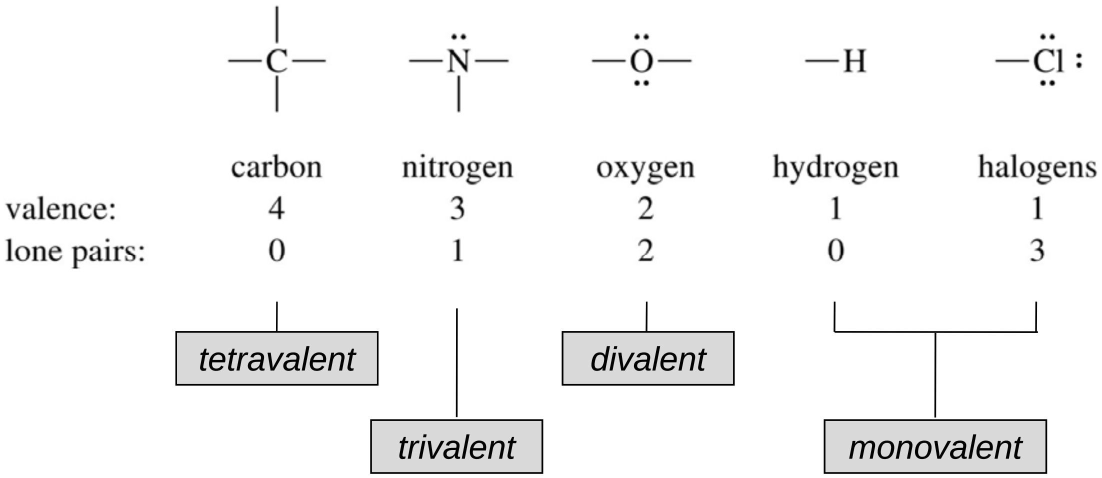
For $2s^2 2p^6$ or $3s^2 3p^6$ elements, this shell has 8 electrons. (Thus “octet”.)

H ($1s^1$) only needs 2 electrons.

Lewis Dash-Bond Structures: Bonds illustrated by lines. (Lone pairs stay dots.)

Typical Valencies and Bonding Patterns

Bonding configurations that fill octets:



	carbon	nitrogen	oxygen	hydrogen	halogens
valence:	4	3	2	1	1
lone pairs:	0	1	2	0	3

Practice Drawing Chemical Structures

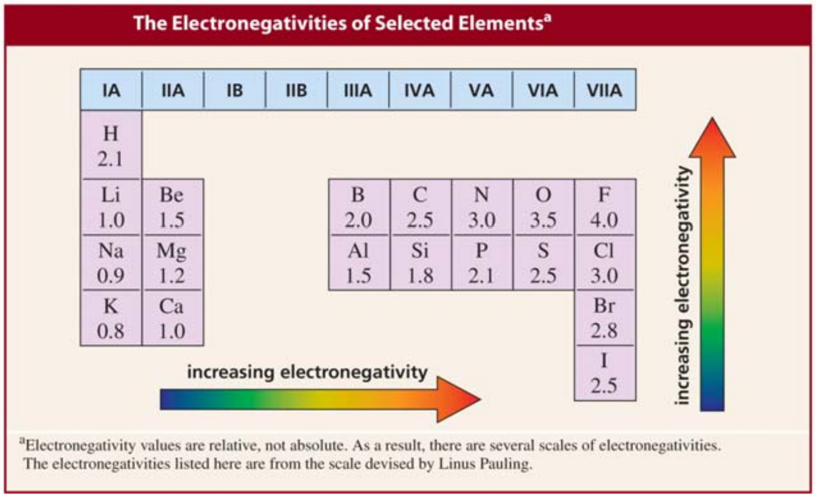
How many ways could you draw C_2H_5N? Try two.

Lewis Dash-Bond Structures:

Line-Angle Structures:

Write carbons as vertices;
Omit H's on carbon;
Omit lone pairs on all atoms.

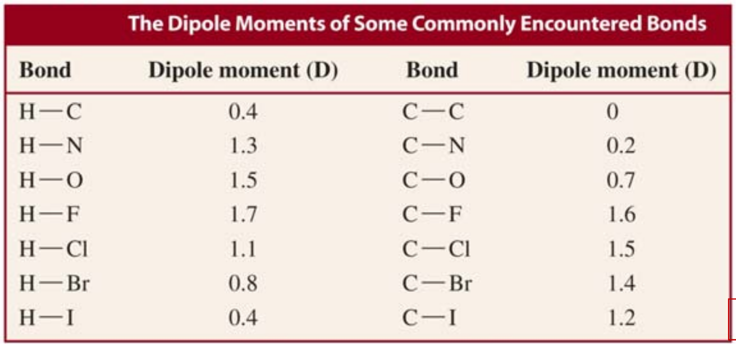
Polar Covalent Bonds



The Electronegativities of Selected Elements[a]

IA	IIA	IB	IIB	IIIA	IVA	VA	VIA	VIIA
H 2.1								
Li 1.0	Be 1.5			B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2			Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0							Br 2.8
								I 2.5

[a] Electronegativity values are relative, not absolute. As a result, there are several scales of electronegativities. The electronegativities listed here are from the scale devised by Linus Pauling.



The Dipole Moments of Some Commonly Encountered Bonds

Bond	Dipole moment (D)	Bond	Dipole moment (D)
H—C	0.4	C—C	0
H—N	1.3	C—N	0.2
H—O	1.5	C—O	0.7
H—F	1.7	C—F	1.6
H—Cl	1.1	C—Cl	1.5
H—Br	0.8	C—Br	1.4
H—I	0.4	C—I	1.2

Electronegativity dictates how equally electrons are "shared" in bonds

Units: Debye (D)

Polar Covalent Bonds

μ = 1.7 D	μ = 1.1 D	μ = 0.8 D	μ = 0.4 D
⟼	⟼	⟼	⟼
H — F	H — Cl	H — Br	H — I

δ+ δ-

partial positive charge

partial negative charge

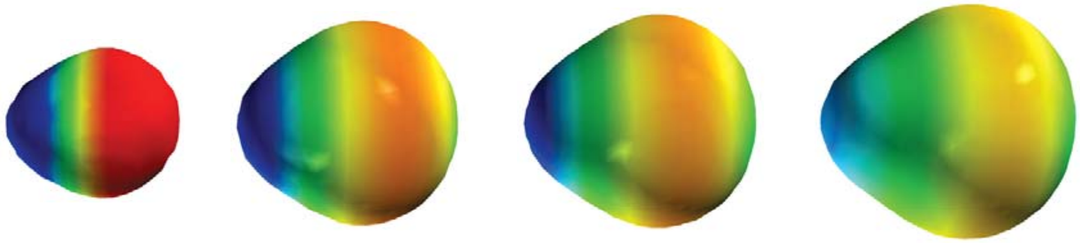
These molecules are neutral, but show regions of charge.

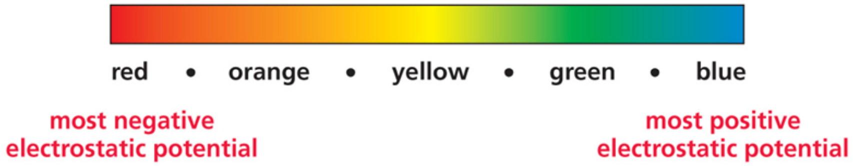
Polar Covalent Bonds

μ = 1.7 D	μ = 1.1 D	μ = 0.8 D	μ = 0.4 D
⟼	⟼	⟼	⟼
H — F	H — Cl	H — Br	H — I

δ+ δ-

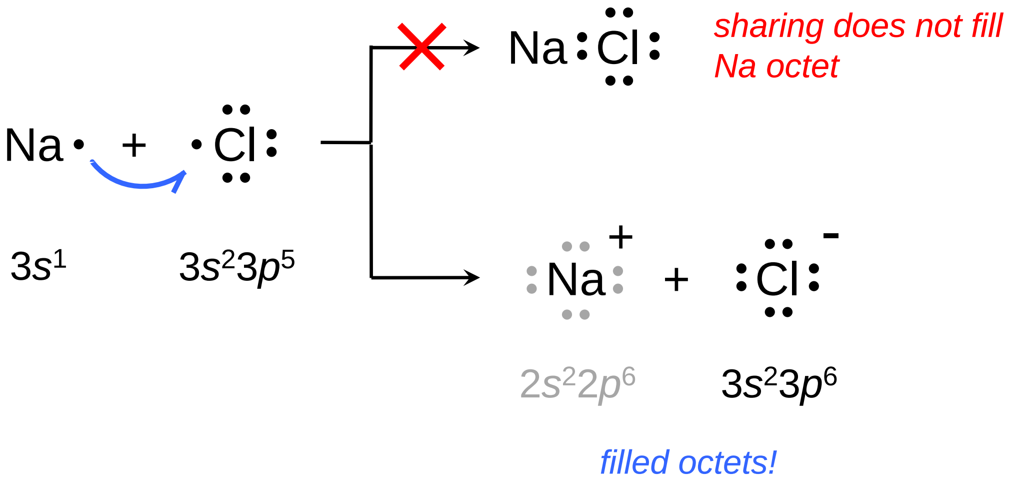
Electrostatic Potential Maps:





These molecules are neutral, but show regions of charge.

Ionic Species: When Atoms Don’t Share

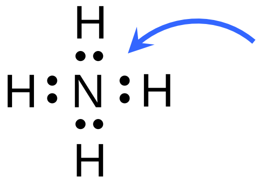


Works because of the large difference in electronegativity between Na and Cl.

Formal Charge in Organic Structures

Formal Charge: Difference between number of valence electrons and “owned” electrons.

$$= (\#\text{ valence } e^-) – (\#\text{ lone pair } e^-) – ½(\#\text{ bonding } e^-)$$



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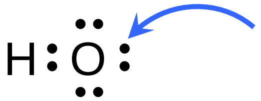
dash-bond structures



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Tip: When # of bonds varies from typical valency, atom is probably charged.

Resonance Structures

Resonance Forms: For a given molecular structure, different ways of placing electrons.

Example: How would you draw $[(CH_3)_2COH]^+$?

What are positive, negative features of these resonance forms?

What are positive, negative features of these resonance forms?

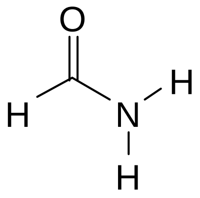
What does this mean for electronic distribution in molecule?

Resonance Structures

- Resonance structures are related by pushing pairs of electrons—lone pairs or multiple bonds—from one location to an adjacent location.
- So, wherever there is a lone pair or a multiple bond, there is the opportunity for resonance.

Resonance rules of thumb:

1. Filled octets are better than unfilled.
   (*Note:* Cannot over-fill octet.)
2. More bonds are better than fewer.
3. Matching charge and electronegativity (+ with electropositive, - with electronegative) is better than mismatching.
4. No charge is better than multiple charges.

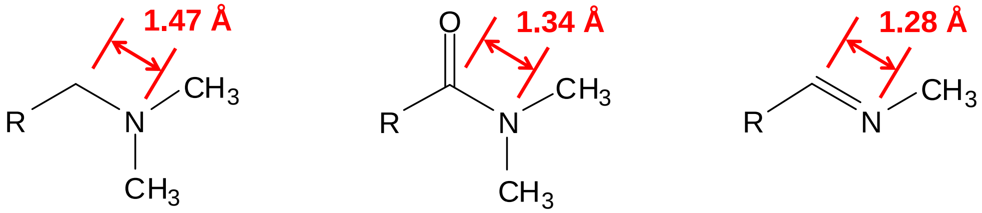


resonance forms?

major or minor?

Resonance and Bond Lengths

Resonance structures explain molecular structures determined by X-ray crystallography.



- Length of C-N bond is between that of typical C-N single and C=N double bonds.
- Bonding must be somewhere in between, consistent with resonance structures.

(C=O is also slightly longer than usual.)