Bonding

Ionic bonding holds ionic compounds (NaCl eg) together

(1) start w/ neutral atoms: $Na_{(g)}$ $Cl_{(g)}$

(2) transfer of valence e⁻: $Na^+_{(g)}$ $Cl^-_{(g)}$

(3) opposite charge ions attract: NaCl

"ionic bond" = electrostatic interaction between opposite charged ions

Covalent bonding involves sharing of valence electrons

Represent with Lewis structures

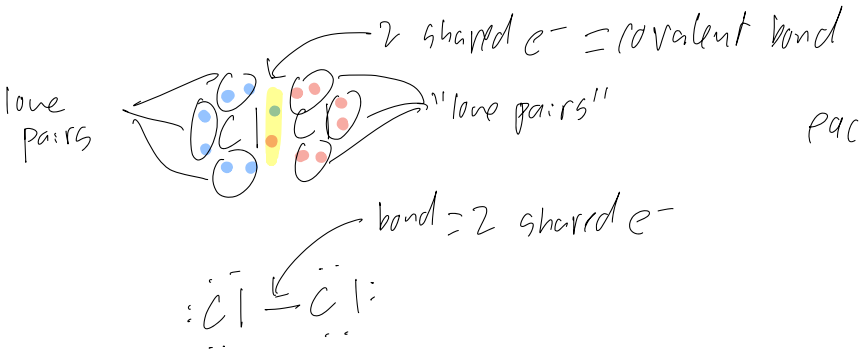
atoms = symbol

electrons = dots

* Most atoms want "octet" – noble gas configuration

Cl_2 molecule has 2 Cl atoms

when 2 Cl atoms get close enough they can share electrons



each Cl has 6 of its "own" e⁻ plus the 2 shared e⁻ = 8 = octet

Going from molecular formula to Lewis structure

(1) Find total # of valence e⁻

(2) Determine atom connectivity

central vs peripheral atoms

H, F, Cl, Br, I tend to only form 1 bond

O, S, Se tend to form 2 bonds
N, P tend to form 3 bonds
C, Si tend to form 4 bonds

(3) connect all atoms with covalent bonds (each bond = 2 e⁻)

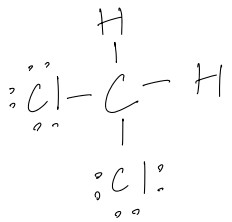
(4) Distribute remaining e⁻ as lone pairs to get atoms to their octet * H atom only needs 2e⁻

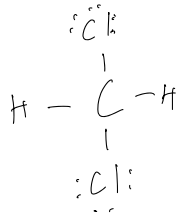
(5) Check – account for all e⁻
– octet/duet

(6) If some atoms "unhappy" try additional bonds

$CH_2Cl_2 \rightarrow 20e^-$

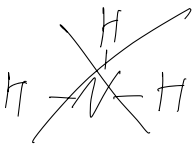
4 2×1 2×7

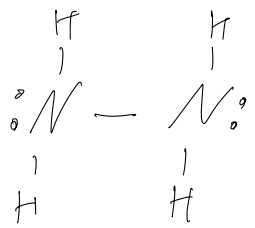




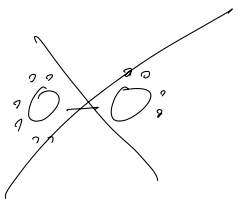
$N_2H_4 \rightarrow 14e^-$

2×5 4×1

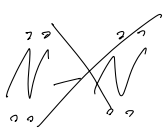


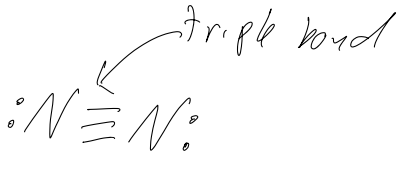


$O_2 \rightarrow 12e^-$



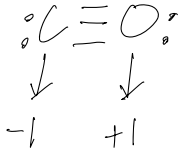
$N_2 \rightarrow 10e^-$

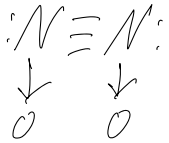




$CO \rightarrow 10e^-$

4 6





Formal charge of atom
– bisect each bond and assign le⁻ to each atom
– add # e⁻ in lone pairs
– compare # e⁻ to # e⁻ on solo atom

non-zero formal charge → unhappy molecule
→ reactive molecule

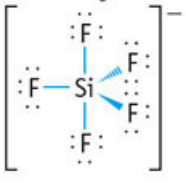
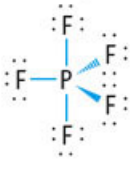
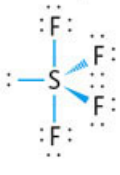
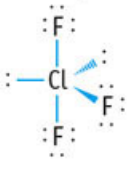
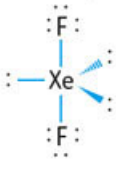
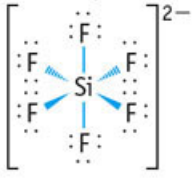
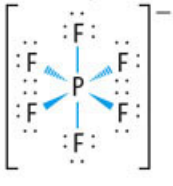
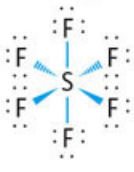
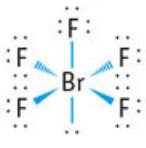
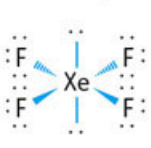
H – only needs 2e⁻

B – only needs 6e⁻

– farther down table
larger atoms – valence e⁻

– farther from nucleus

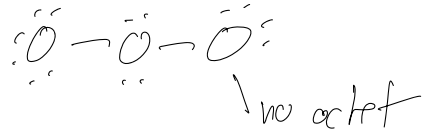
TABLE 8.6 Lewis Structures in Which the Central Atom Exceeds an Octet

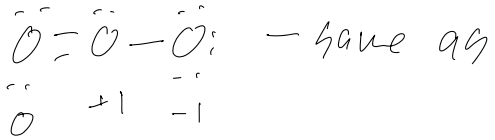
Group 4A	Group 5A	Group 6A	Group 7A	Group 8
SiF_5^- 	PF_5 	SF_4 	ClF_3 	XeF_2 
SiF_6^{2-} 	PF_6^- 	SF_6 	BrF_5 	XeF_4 

Resonance

O_3 - ozone - 18e

- doesn't actually work

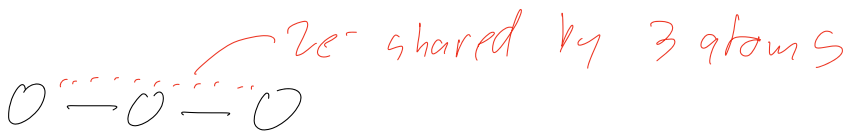




Expect asymmetric molecule b/c 1 side has double bond and 1 side has single bond

Experiments show that molecule is symmetric

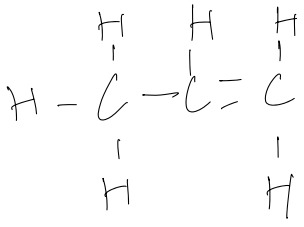
2 electrons shared by all 3 atoms

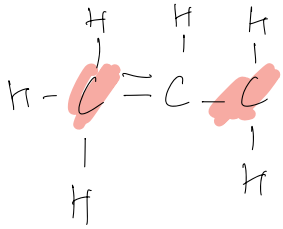


[O - O=O O=O-O] - 2 resonance structures

("reality" is the average of the resonance structures)

Need double bond that can be put in multiple locations without moving any atoms





← Not resonance

3D structure described by Valence Shell Electron Pair Repulsion (VSEPR)

* electron pairs repel each other and try to avoid each other

Electron pair geometry at each atom is what we need to understand

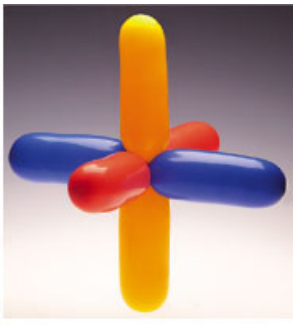
2 e⁻ pairs | 3 e⁻ pairs | 4 e⁻ pairs | 5 e⁻ pairs | 6 e⁻ pairs

Linear

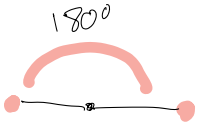
Trigonal planar

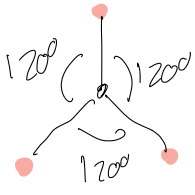
Tetrahedral

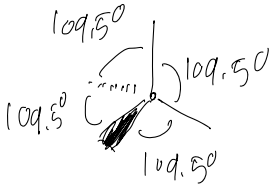
Trigonal bipyramidal



Octahedral







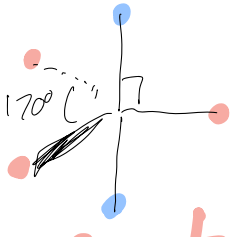
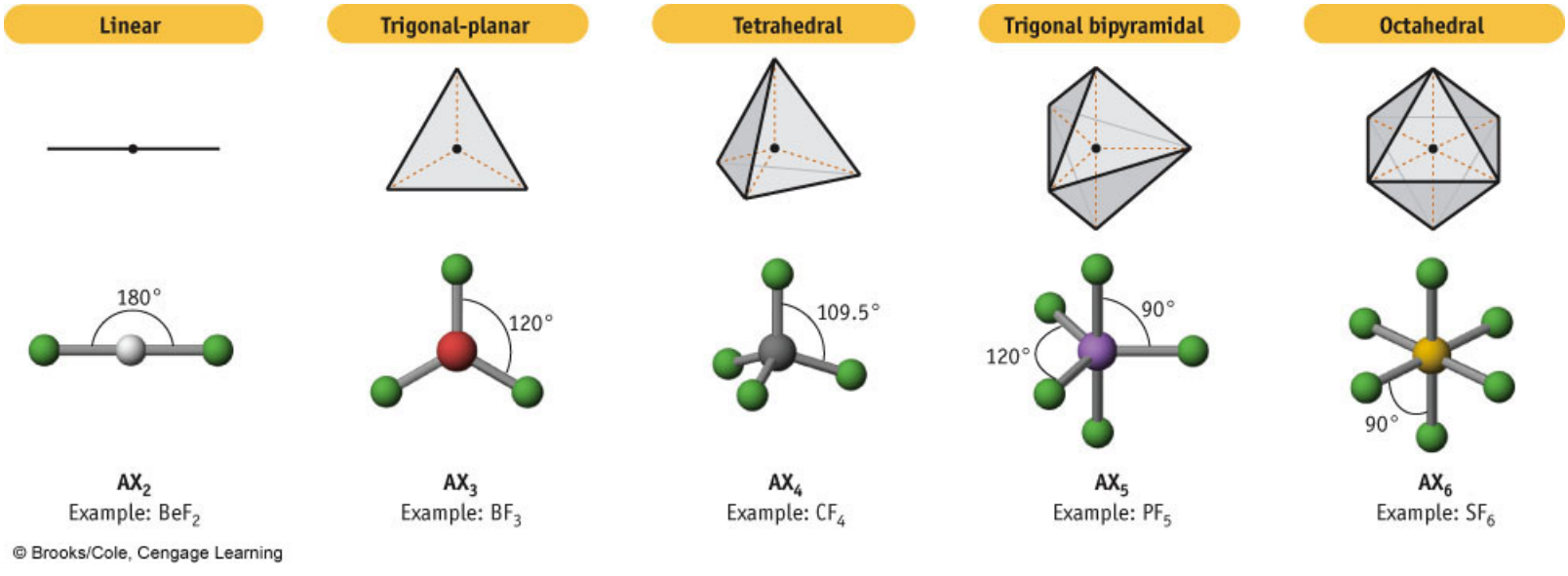


Fig. 8-4, p. 368



Consider all atoms with 1 thing connected to it

- determine # of electron pairs around atom → electron pair geometry

bonds and lone pairs count as electron pairs

molecular geometry is only where atoms are

Fig. 8-5, p. 369

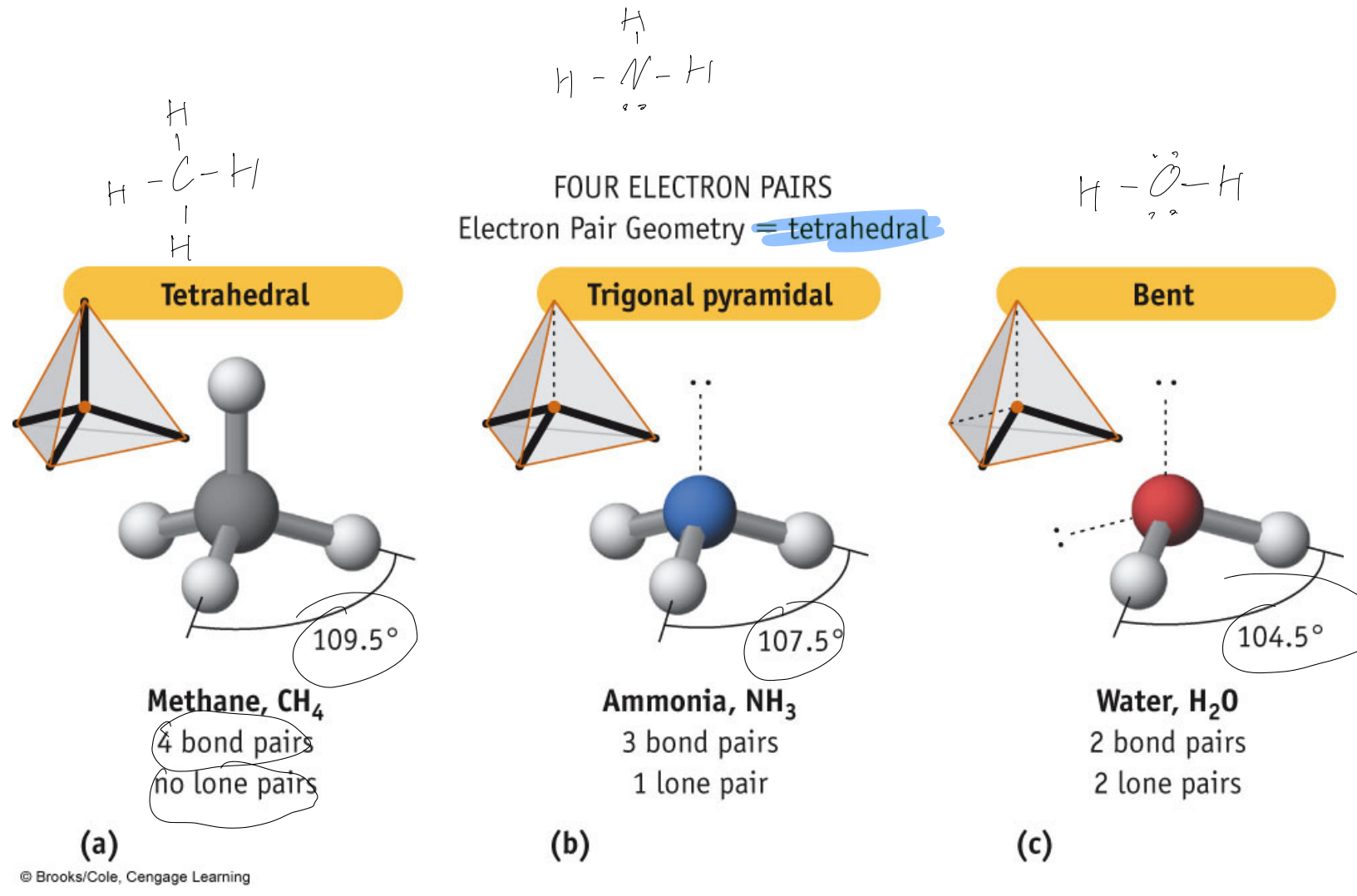


Fig. 8-6, p. 371

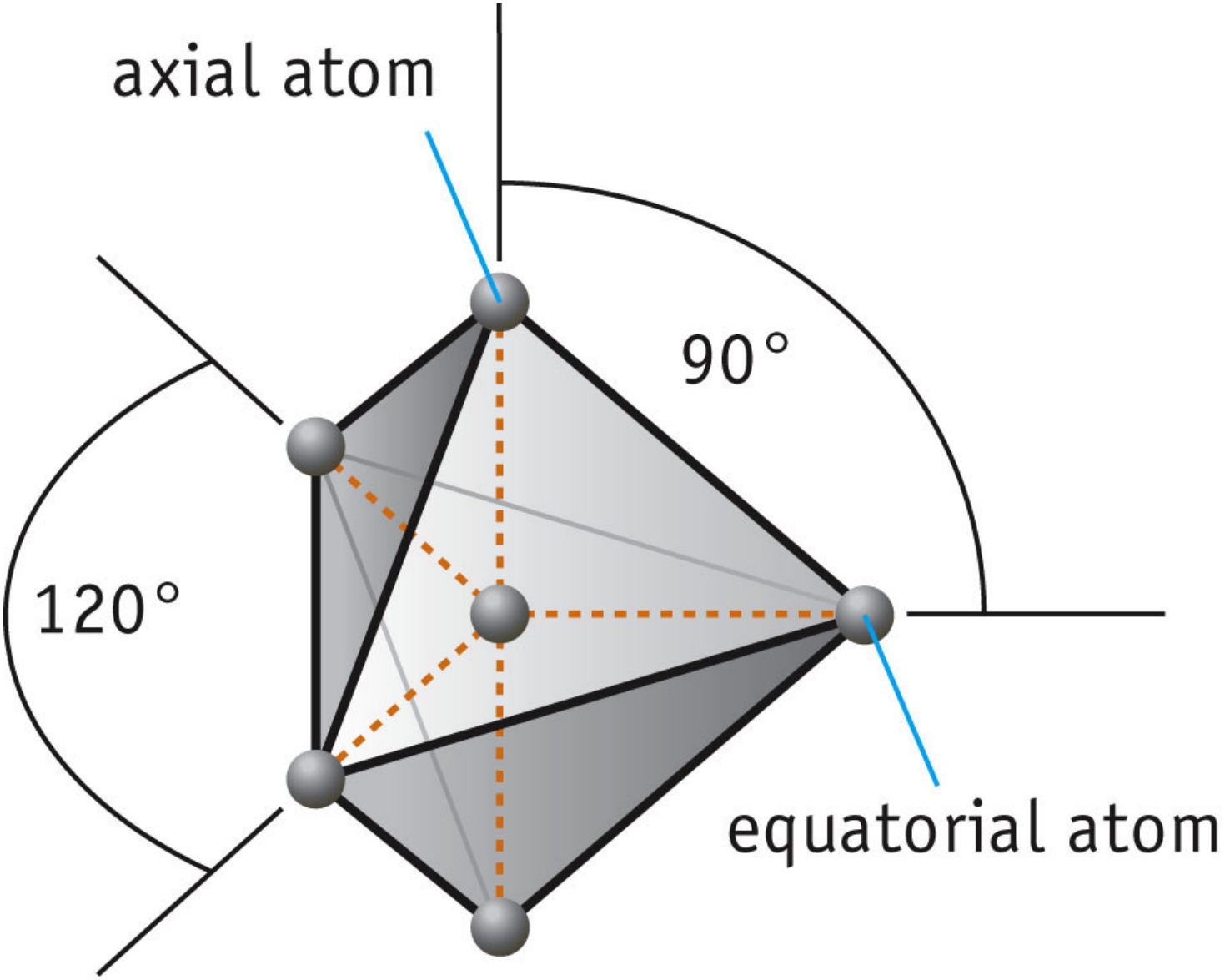
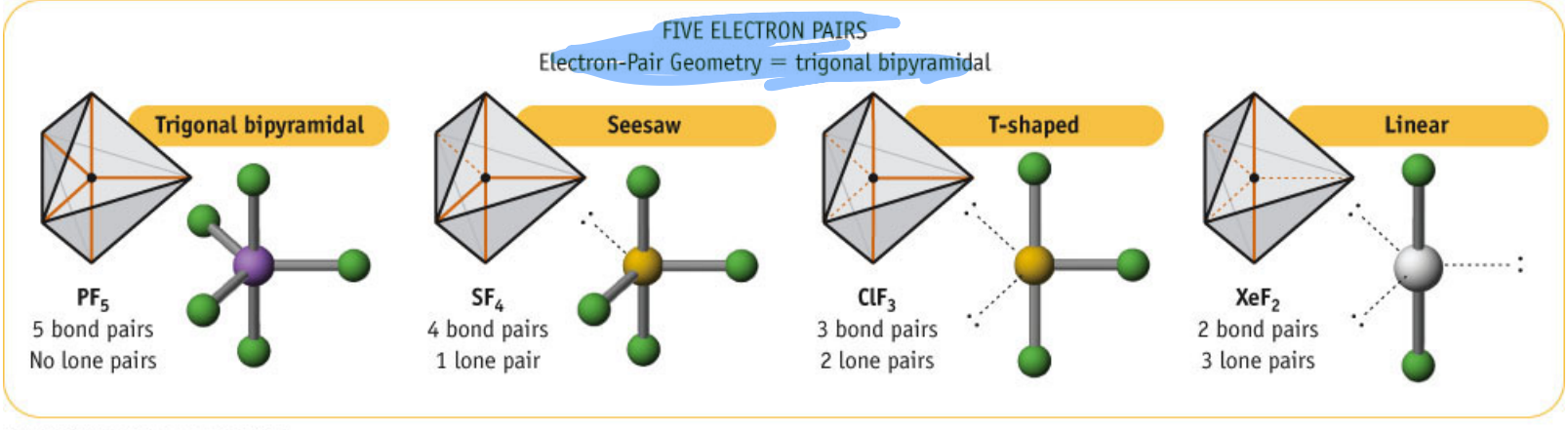


Fig. 8-7, p. 372

* lone pairs always go equatorial



ClF_3 28 e⁻

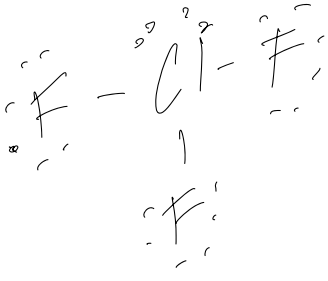
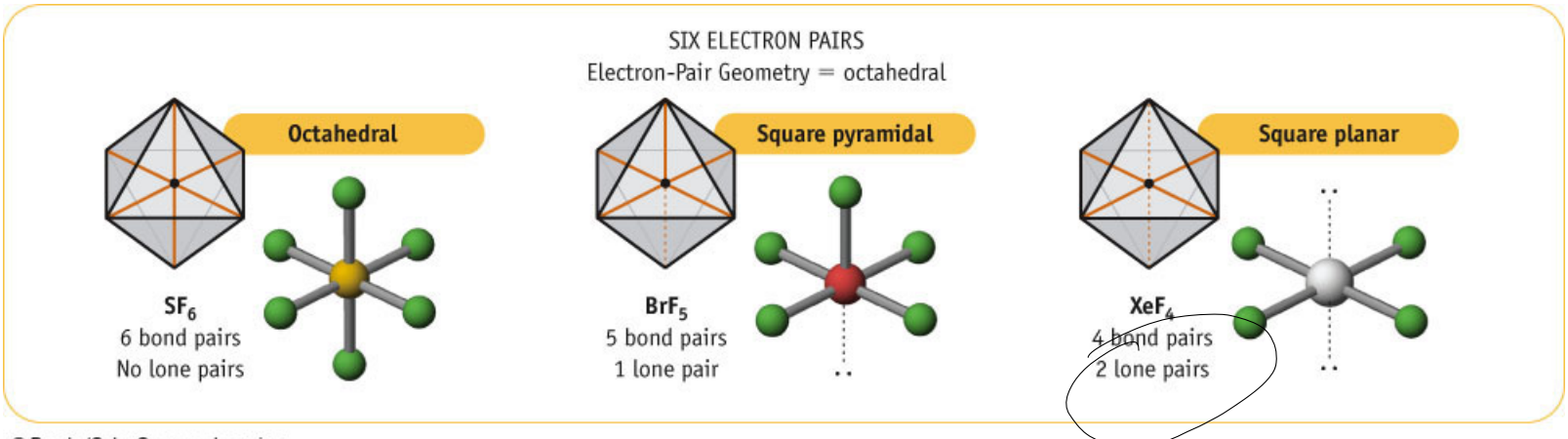


Fig. 8-8, p. 372



remove bond opposite of where you put lone pair

Fig. 8-8, p. 372

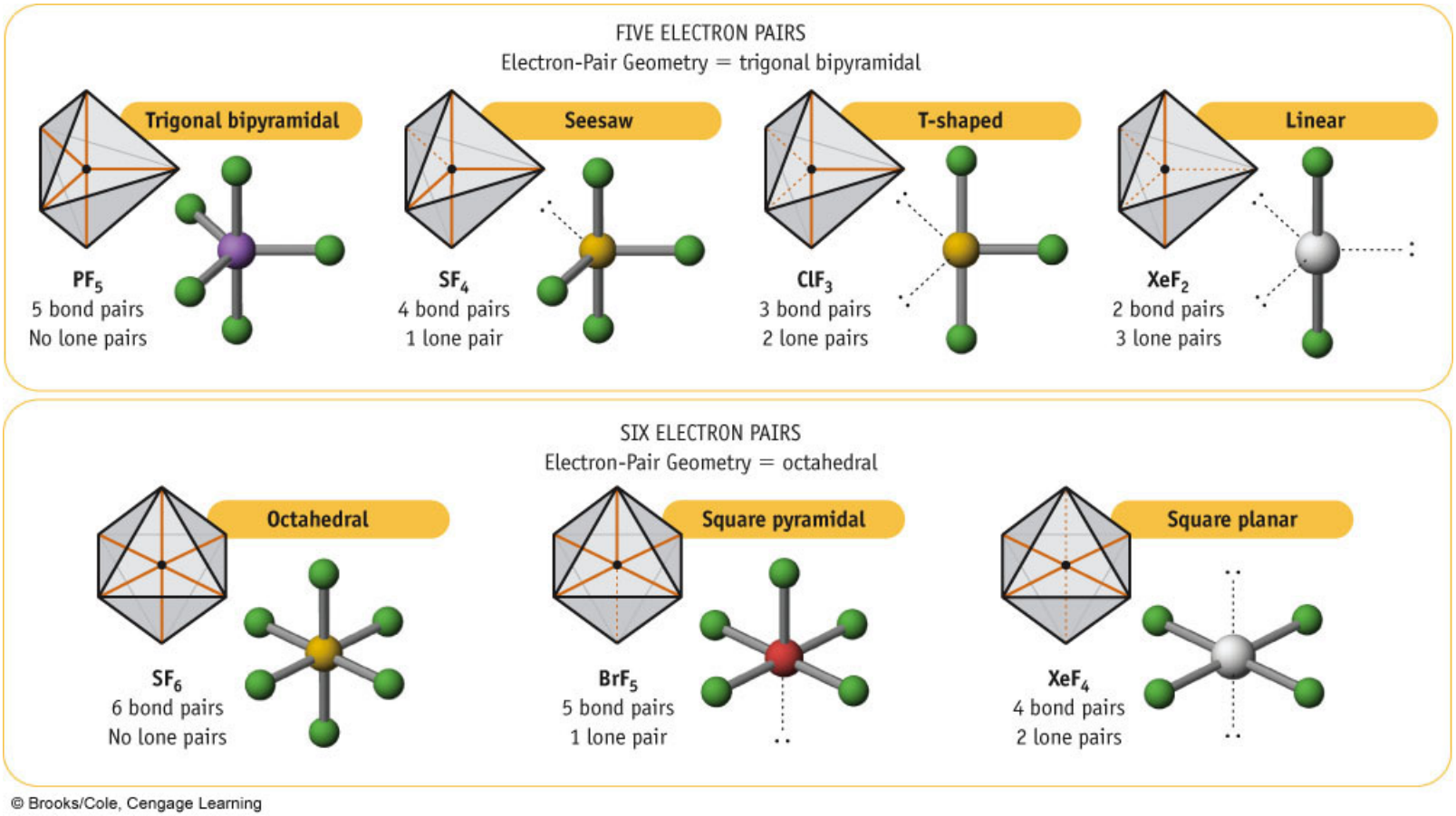
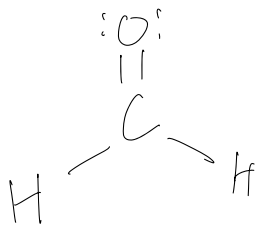


Fig. 8-8, p. 372

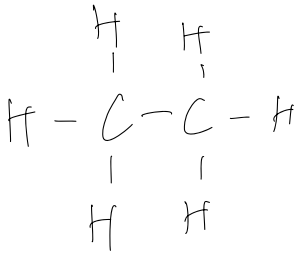
For double/triple bonds in 3D structures "count" as only 1 pair of electrons

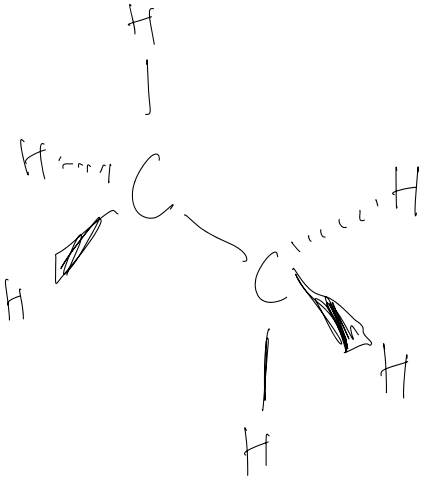
- 3 e⁻ pairs - all bonds

→ trigonal planar



CH_3CH_3





Ideal covalent bond has perfectly equitable sharing of electron pair

most of time electrons are shared unequally resulting in one end of bond with more electron density and one end with less → Polar bond

Electronegativity - how selfish an atom is about sharing electrons 0 → 4

least selfish (0) · most selfish (4)

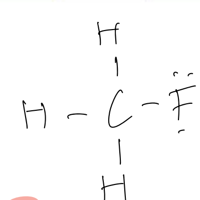
If Δ electroneg btw 2 atoms is ≥ 0.5 bond is polar

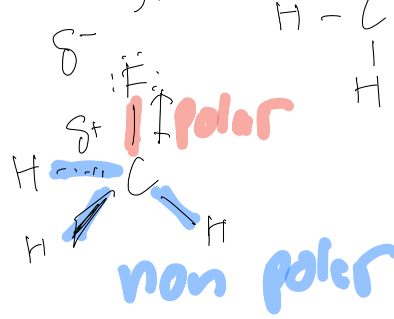
H 2.2

1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A
Li 1.0	Be 1.6											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.3											Al 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2
K 0.8	Ca 1.0	Sc 1.4	Ti 1.5	V 1.6	Cr 1.7	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.8	Ge 2.0	As 2.2	Se 2.6	Br 3.0
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.3	Nb 1.6	Mo 2.2	Tc 1.9	Ru 2.2	Rh 2.3	Pd 2.2	Ag 1.9	Cd 1.7	In 1.8	Sn 2.0	Sb 1.9	Te 2.1	I 2.7
Cs 0.8	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5	W 2.4	Re 1.9	Os 2.2	Ir 2.2	Pt 2.3	Au 2.5	Hg 2.0	Tl 1.6	Pb 2.3	Bi 2.0	Po 2.0	At 2.2

<1.0 · 1.0–1.4 · 1.5–1.9 · 2.0–2.4 · 2.5–2.9 · 3.0–4.0

CH_3F





δ+ δ− partial charges

pos → neg

Fig. 8-11, p. 376

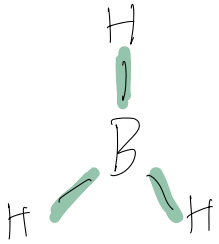
more electroneg atom is the negative end of the bond

Polar bonds can lead to polar molecules

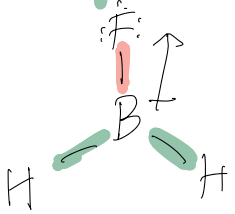
polar bond
non polar bonds

BH_3
BH_2F
BHF_2
BF_3

B eneg = 2.0
H eneg = 2.2
F eneg = 4.0



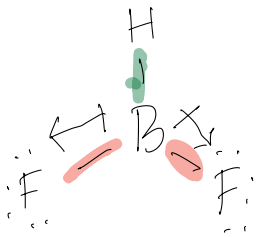
non polar molecule



polar molecule

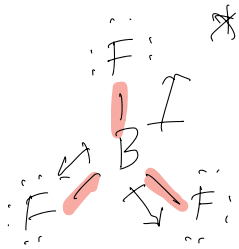
look at each bond polarity

how does sum of all cancel or not cancel

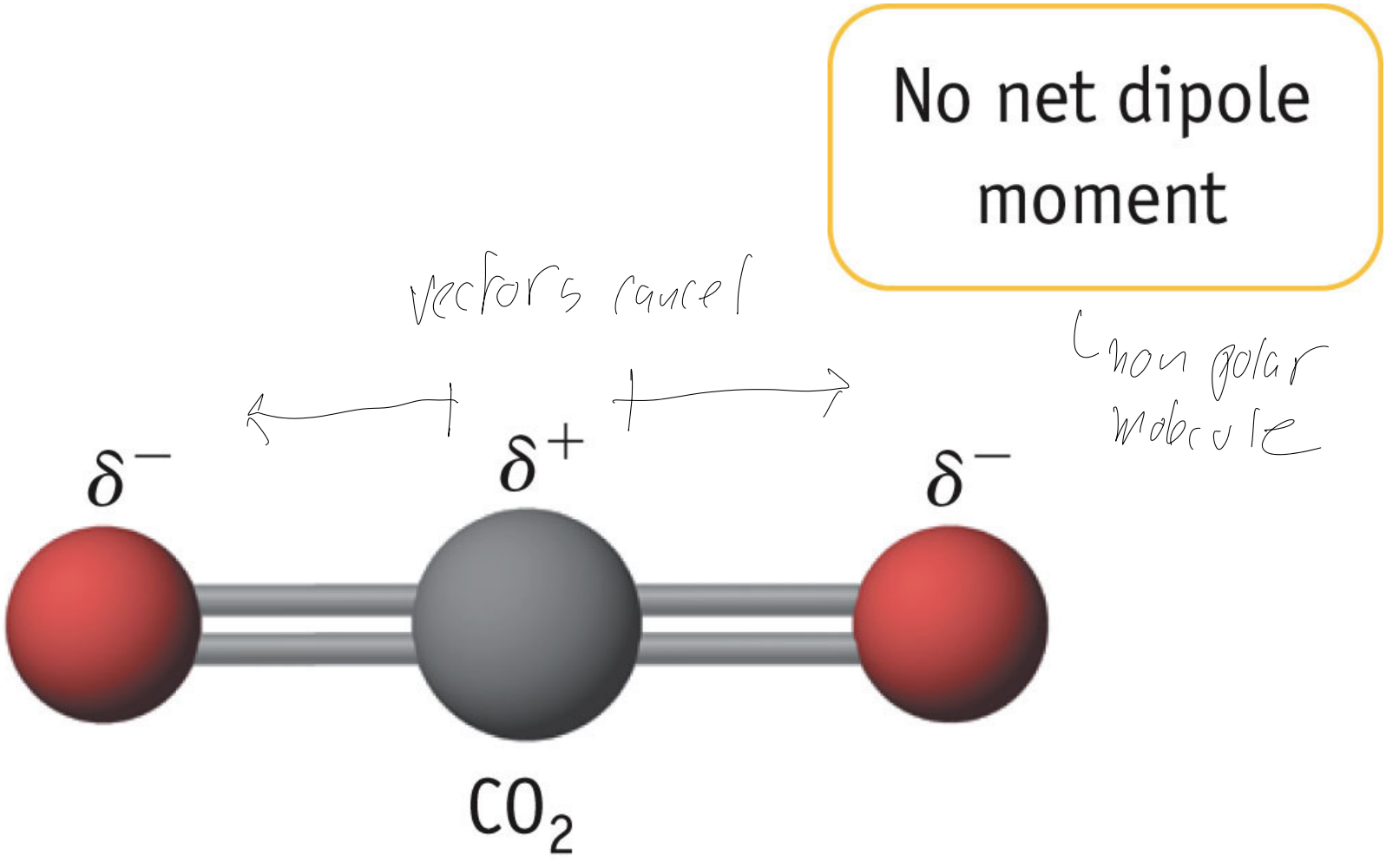


polar molecule

* vectors cancel

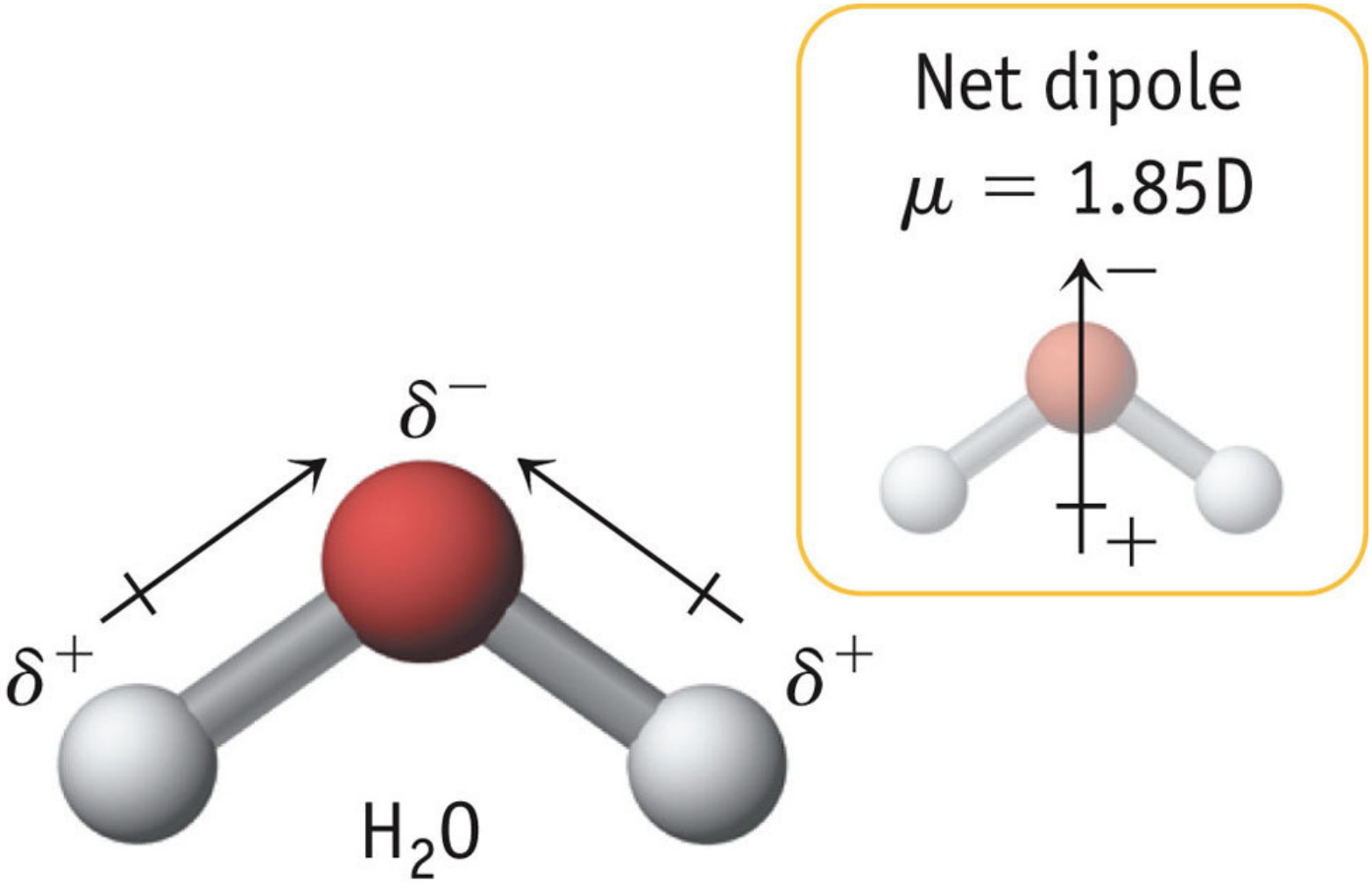


non polar molecule



(a)

Fig. 8-13, p. 381



(b)

Fig. 8-13, p. 381

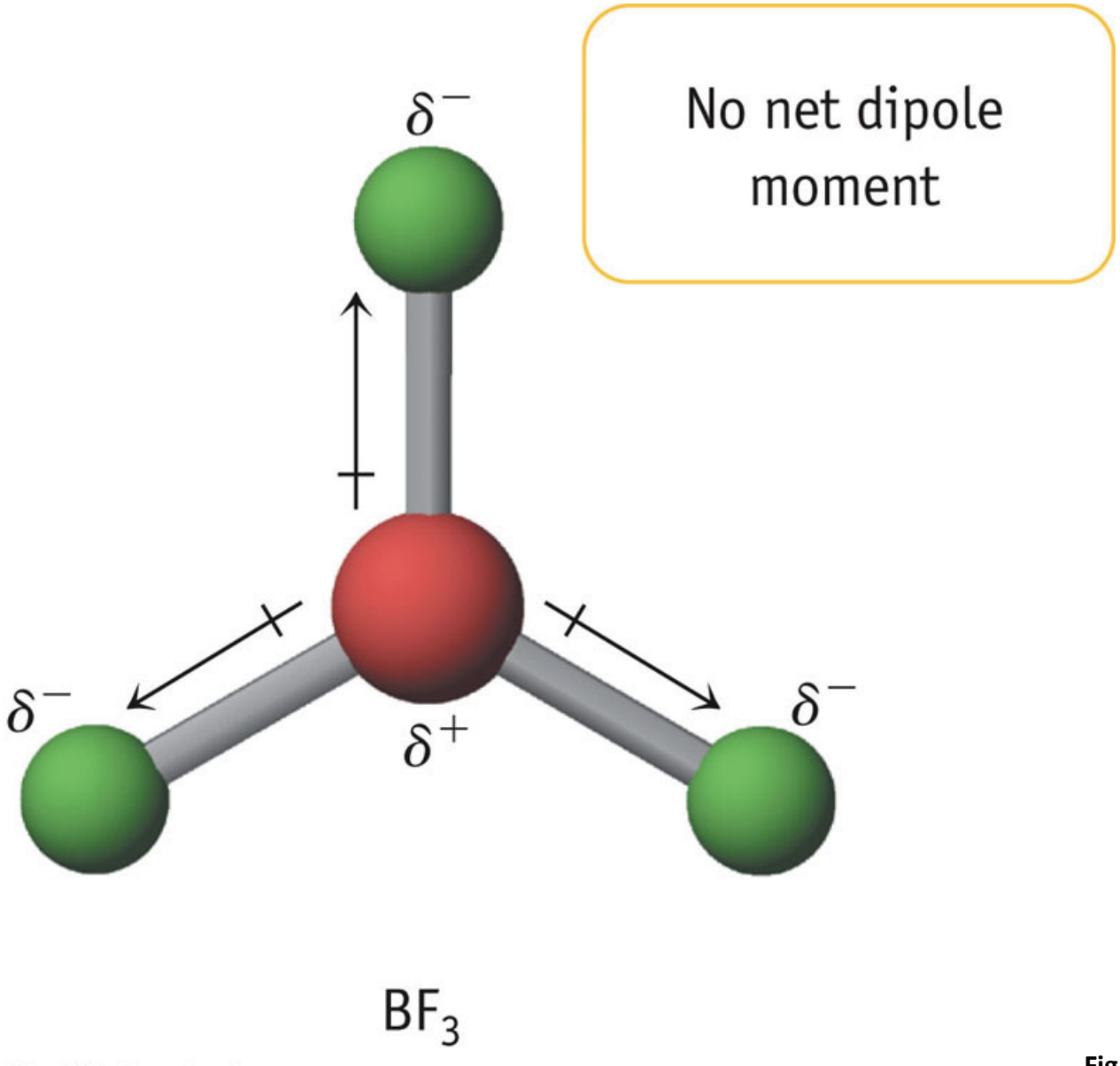


Fig. 8-14, p. 383

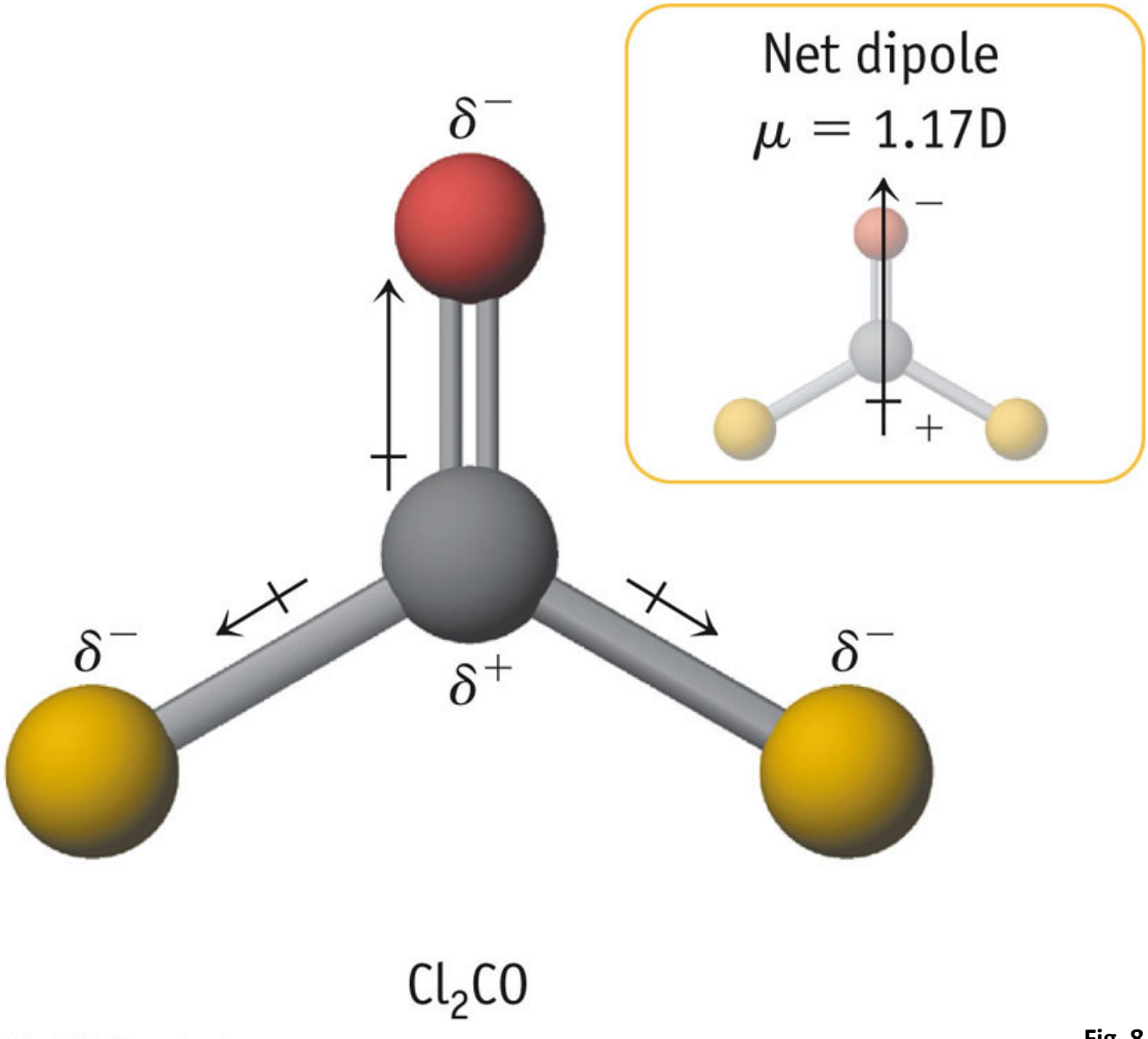
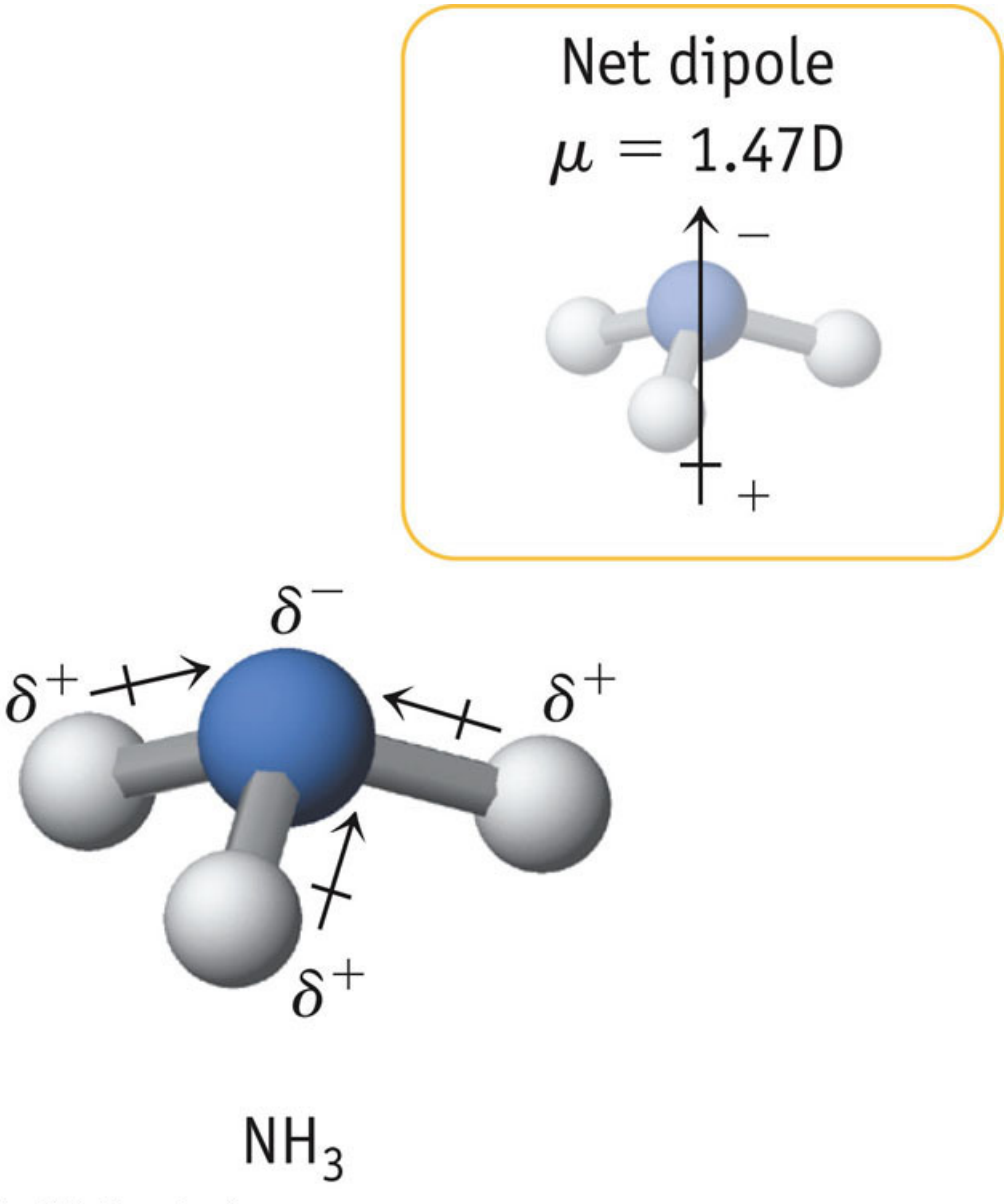


Fig. 8-14, p. 383



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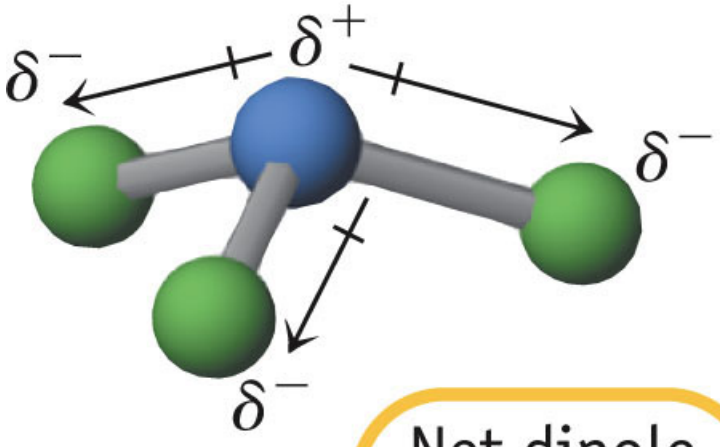
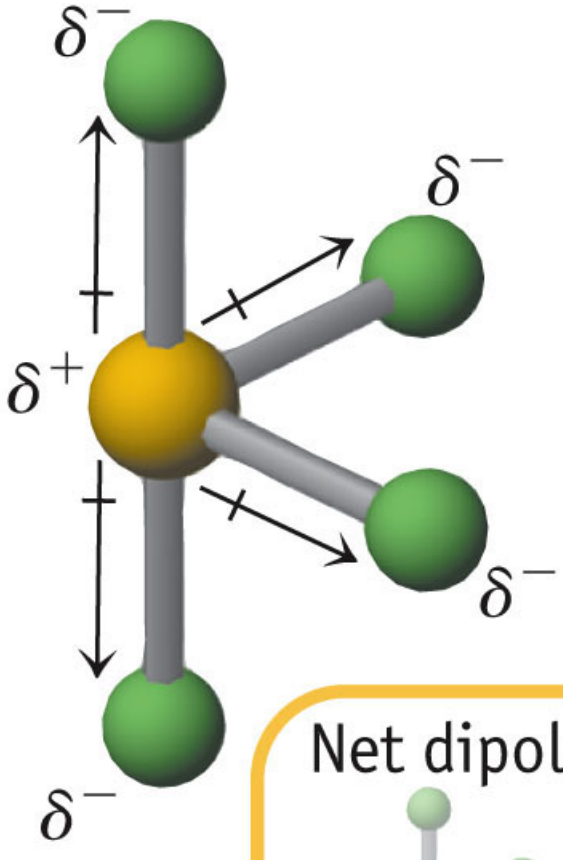
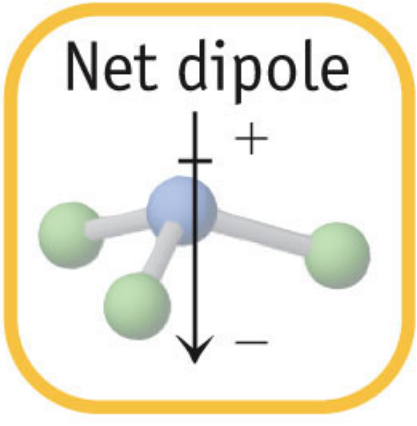
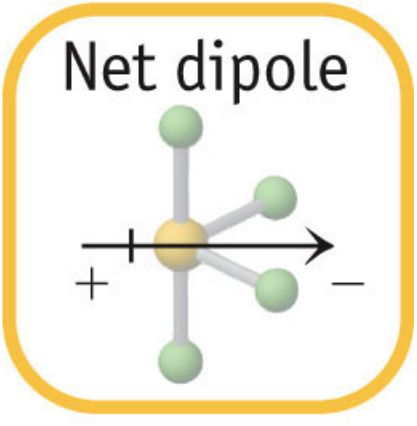




NF_3



SF_4



Example 8-12, p. 384

TABLE 8.8 Some Average Single- and Multiple-Bond Lengths in Picometers (pm)*

Single Bond Lengths

	Group 1A	4A	5A	6A	7A	4A	5A	6A	7A	7A	7A
	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

Multiple Bond Lengths

C═C	134	C≡C	121
C═N	127	C≡N	115
C═O	122	C≡O	113
N═O	115	N≡O	108

*1 pm = 10^{-12} m.

Table 8-8, p. 387

TABLE 8.9 Some Average Bond Dissociation Enthalpies (kJ/mol)*

Single Bonds

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	413	391	463	565	328	322	347	432	366	299
C		346	305	358	485	—	—	272	339	285	213
N			163	201	283	—	—	—	192	—	—
O				146	—	452	335	—	218	201	201
F					155	565	490	284	253	249	278
Si						222	—	293	381	310	234
P							201	—	326	—	184
S								226	255	—	—
Cl									242	216	208
Br										193	175
I											151

Multiple Bonds

N═N	418	C═C	610
N≡N	945	C≡C	835
C═N	615	C═O	745
C≡N	887	C≡O	1046
O═O (in O_2)	498		

*Sources of dissociation enthalpies: I. Klotz and R. M. Rosenberg: *Chemical Thermodynamics*, 4th Ed., p. 55, New York, John Wiley, 1994; and J. E. Huheey, E. A. Keiter, and R. L. Keiter: *Inorganic Chemistry* 4th Ed., Table E. 1, New York, Harper-Collins, 1993. See also Lange's *Handbook of Chemistry*, J. A. Dean (ed.), McGraw-Hill Inc., New York.

Table 8-9, p. 389