11/28/18

Bond Energies + ΔH_{rxn}

Cost E (+) to break bonds
Releases E (-) to make bonds.

table of avg bond enthalpies

Bond	Bond "energy" (ΔH, KJ/mol)
C–C	347
C=C	611
N≡N	946
N–H	389
H–H	436

Can use this info to predict ΔH_{rxn}.

How? $\Delta H_{rxn} = \underbrace{\sum \text{Bonds broken}}_{(+)\text{ costs E}} \underbrace{\ominus \sum \text{Bonds made}}_{(-)\text{ releases E}}$

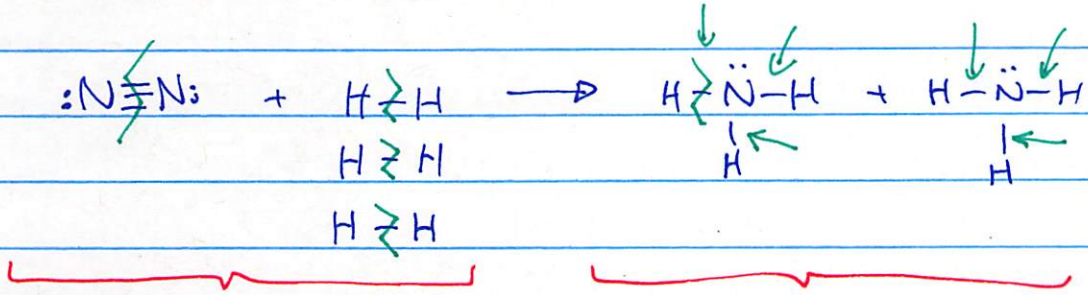
TABLE 9.3 Average Bond Energies

Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)
H—H	436	N—N	163	Br—F	237
H—C	414	N=N	418	Br—Cl	218
H—N	389	N≡N	946	Br—Br	193
H—O	464	N—O	222	I—Cl	208
H—S	368	N=O	590	I—Br	175
H—F	565	N—F	272	I—I	151
H—Cl	431	N—Cl	200	Si—H	323
H—Br	364	N—Br	243	Si—Si	226
H—I	297	N—I	159	Si—C	301
C—C	347	O—O	142	S—O	265
C= C	611	O=O	498	Si=O	368
C≡C	837	O—F	190	S=O	523
C—N	305	O—Cl	203	Si—Cl	464
C=N	615	O—I	234	S=S	418
C≡N	891	F—F	159	S—F	327
C—O	360	Cl—F	253	S—Cl	253
C=O	736*	Cl—Cl	243	S—Br	218
C≡O	1072			S—S	266
C—Cl	339				

*799 in CO_2.

ex: $N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$

Draw Lewis:



Break (+) Bonds

Make (−) Bonds

$\Delta H_{rxn} \approx (1\,mol \times N\equiv N + 3\,mol \times H-H) \ominus (6\,mol \times N-H)$

$\approx \left(1\,mol \times 946\frac{kJ}{mol} + 3\,mol \times 436\frac{kJ}{mol}\right) \ominus \left(6\,mol \times 389\,kJ/mol\right)$

$\approx -80.\,kJ$ (xpt: $\Delta H_{rxn} = -91.8\,kJ$)

Chapter 10: Chemical Bonding 2

Shapes of molecules ~ determines function + props

Simple model to predict 3-D shapes: VSEPR

VSEPR = Valence Shell Electron Pair Repulsion

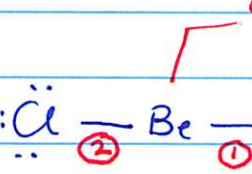
e⁻ pairs repel // try to stay far apart!

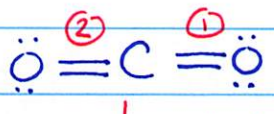
- Bonds (single, double, or triple)
- lone-pairs

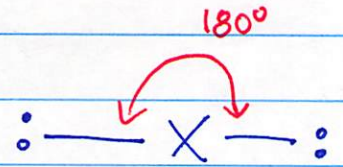
- Consider a central atom + count # bonds + lone-pairs (any type)

2-repulsions

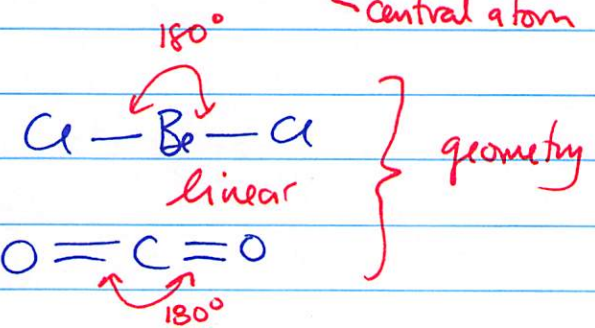
such as: central atom

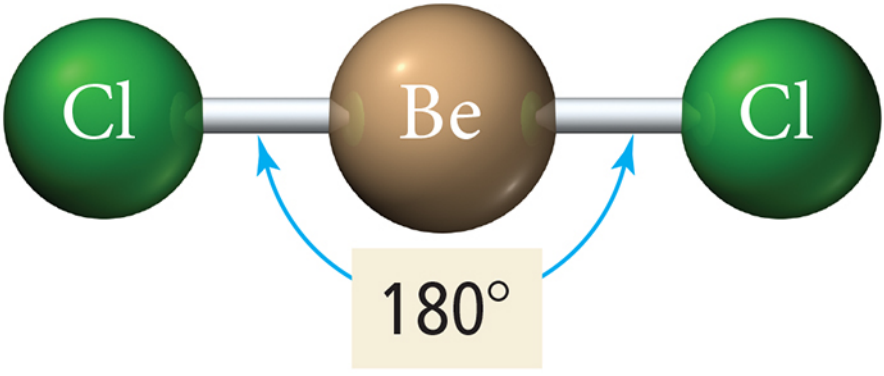






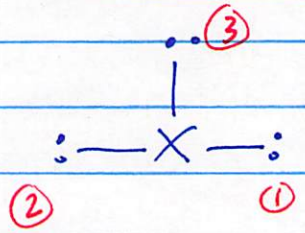
name: linear



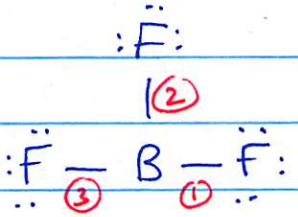


(a) Linear geometry

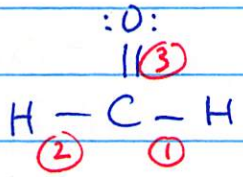
3-repulsions

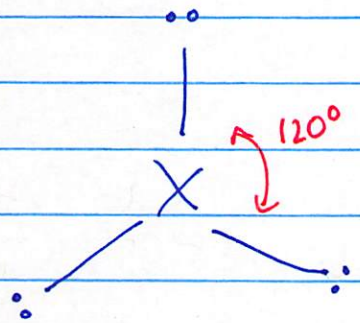


such as:

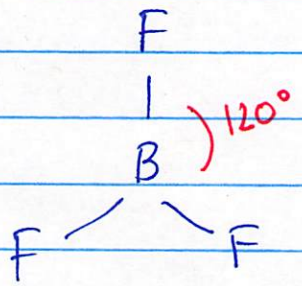


or

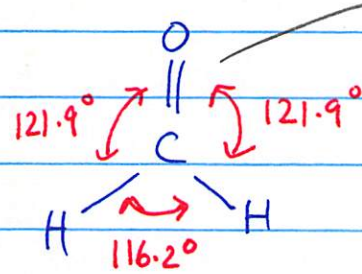




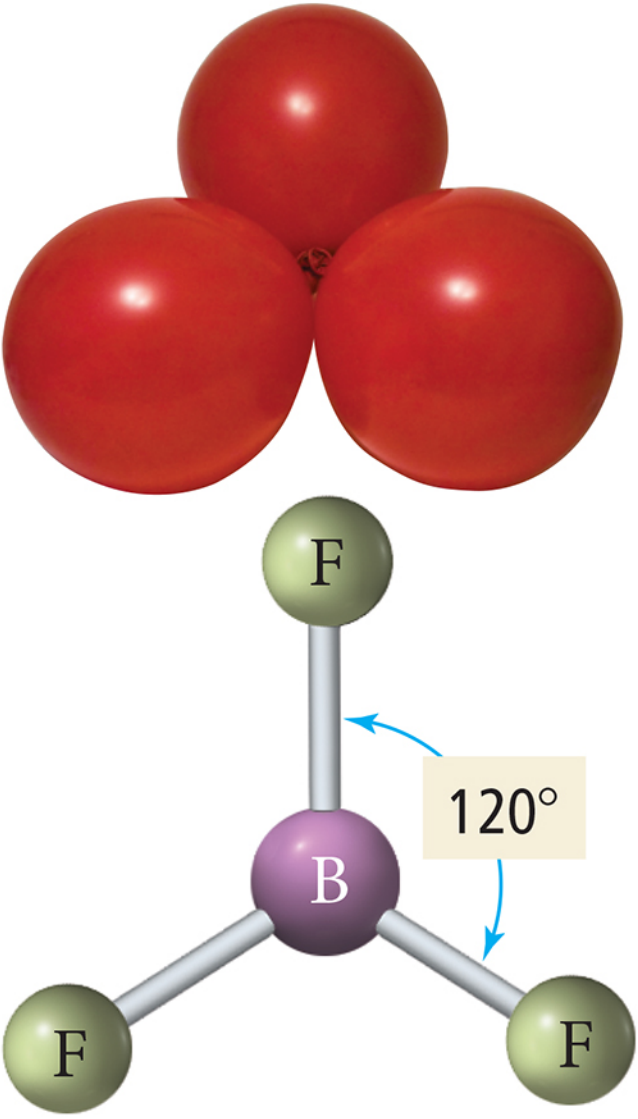
name: trigonal-planar



trigonal-planar



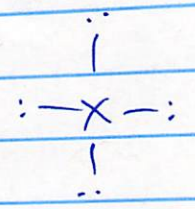
"falter" bond
- more e⁻ density



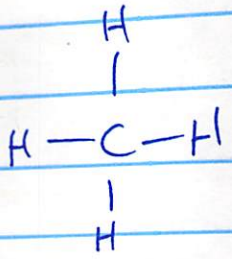
(b) Trigonal planar geometry

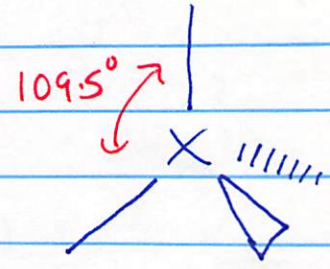
~~4 = pairs~~

4 - repulsions



such as



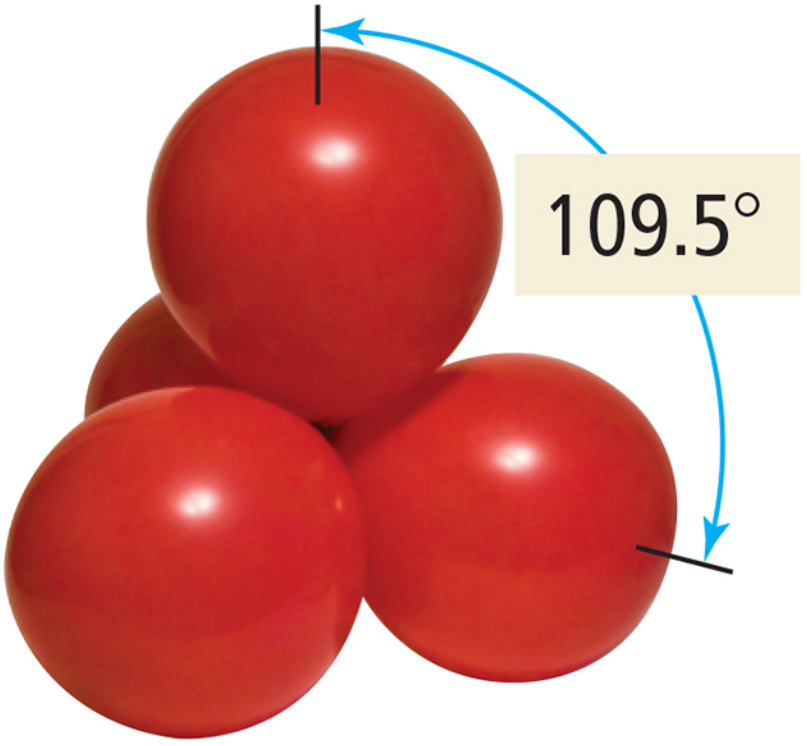


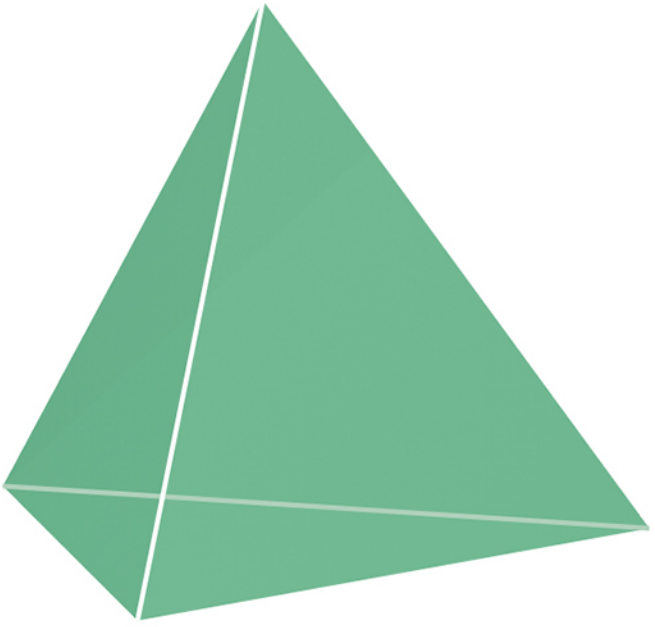
name: tetrahedral.

| = in the plane

△ = out of plane

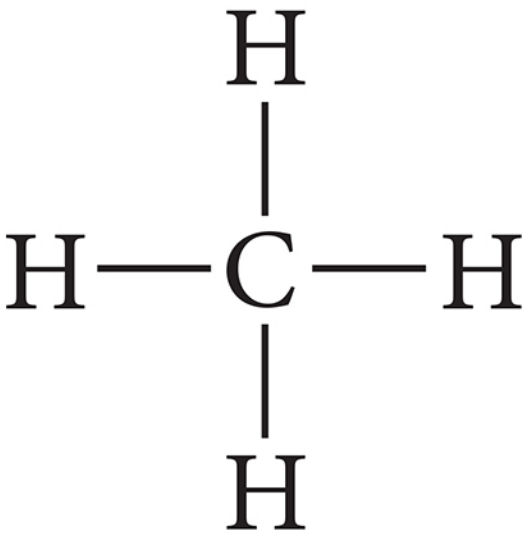
≡ = behind plane

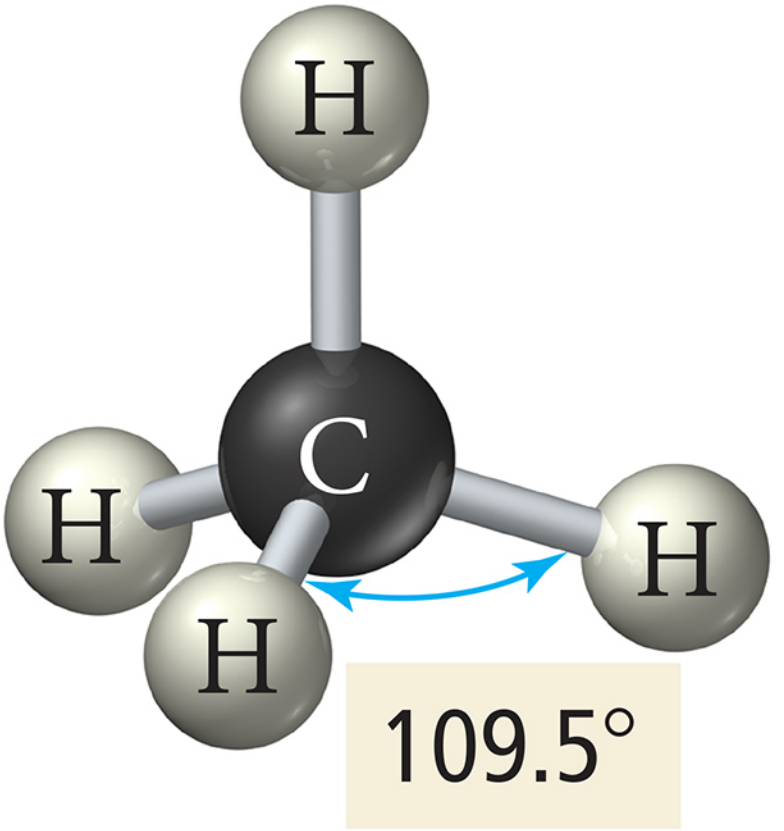




Tetrahedral geometry

Tetrahedron





Tetrahedral geometry