Seřaďte následující molekuly sestupně podle velikosti vazebného úhlu.

(i) SF_6, H_2O, NH_3, CH_4

(ii) NH_3, CH_4, BF_3, $BeCl_2$

(iii) BeH_2, H_2O, $AlCl_3$, H_2S

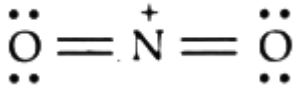
(i) CH_4 (109.5º) > NH_3 (107º) > H_2O (104.5º) > SF_6 (90º)

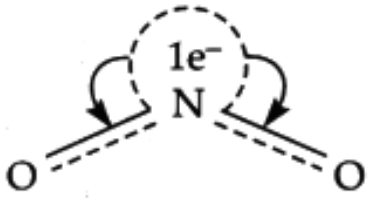
(ii) $BeCl_2$ > BF3 (120º) > CH_4 (109.5º) > NH_3 (107º)

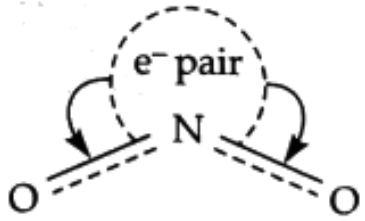
(iii) BeH_2 (108º) > $AlCl_3$ (120º) v > H_2O (104.5º) > H_2S (100º) (S je méně electronegativní a atom S je větší než atom O)

Seřaďte následující molekuly sestupně podle velikosti vazebného úhlu: NO_2, NO_2^+, NO_2^-.

NO_2^+ (180º) > NO_2 (132º) > NO_2^- (115º)



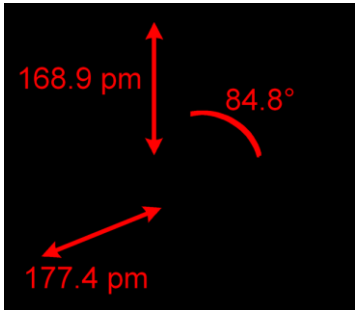


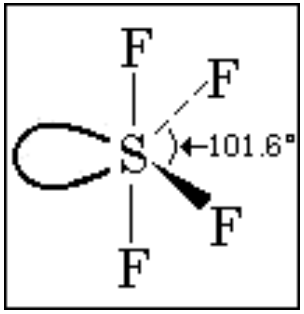


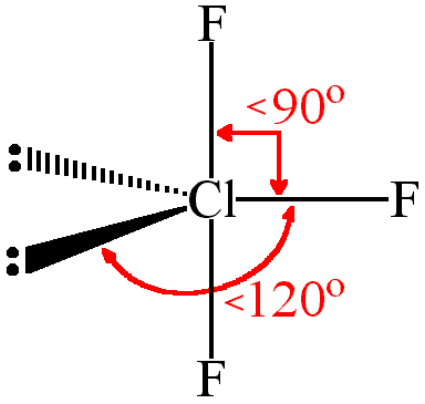
Vysvětlete změny vazebných úhlů X-C-X v molekulách H_2CO, F_2CO a Cl_2CO.

H_2CO (116°) > Cl_2CO (111°) > F_2CO (108°)

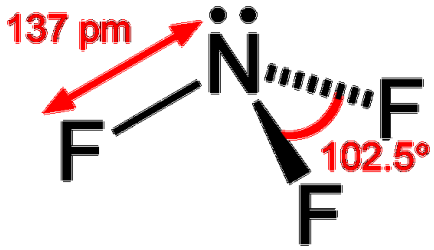
Diskutujte hodnoty vazebných úhlů v BrF_5, SF_4 a ClF_3

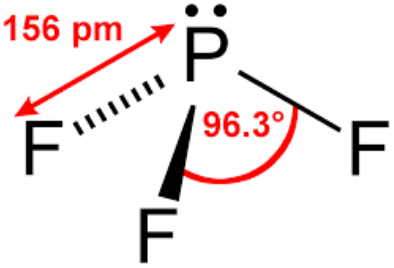






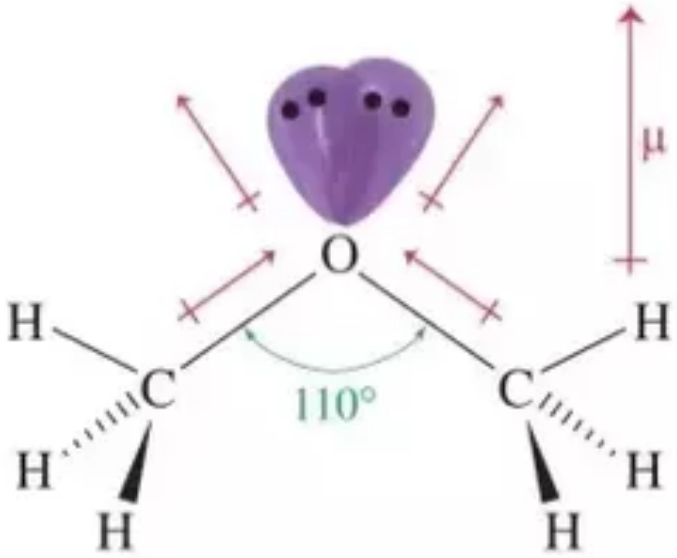
Diskutujte hodnoty vazebných úhlů v NF_3 a PF_3





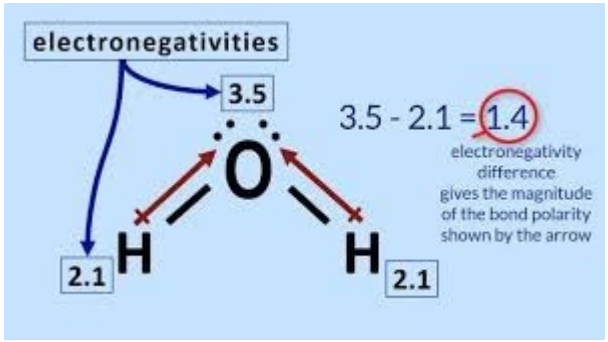
Structure and Polarity

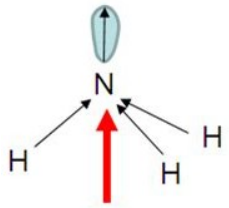
- Oxygen is sp^3 hybridized.
- Bent molecular geometry.
- C—O—C angles is 110°.
- Polar C—O bonds.
- Dipole moment of 1.3 D.



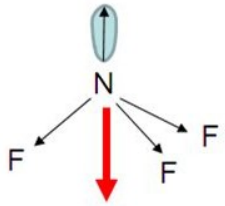
Polarita molekuly, dipólový moment

Dipolový moment molekuly = vektorový součet všech vazebných dipolů. Může být nulový, i v případě nenulových vazebných dipolů které se navzájem kompenzují (např. SF_6, SiF_4, CF_4, …)

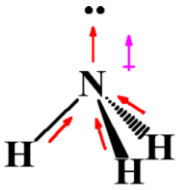




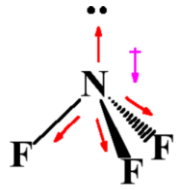
ΔEN = 0.9



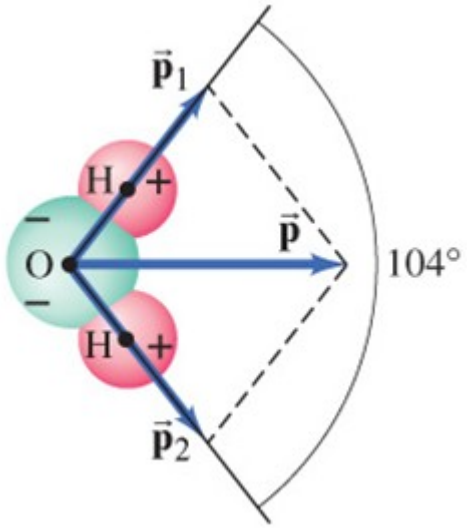
ΔEN = 1

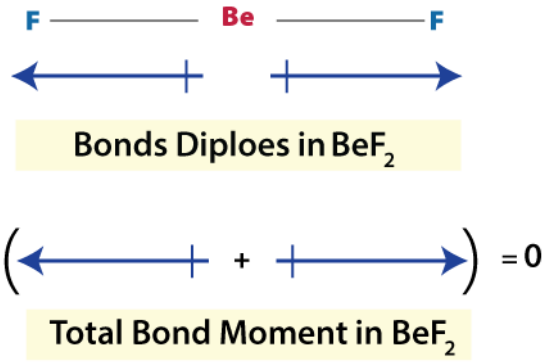


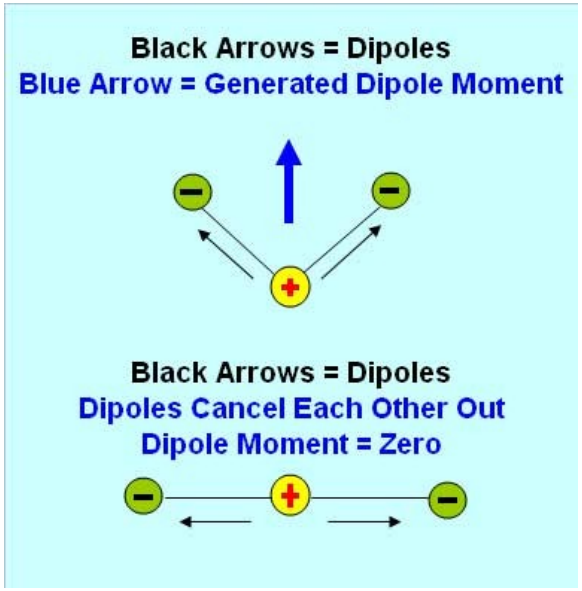
μ = 1.46 D



μ = 0.24 D





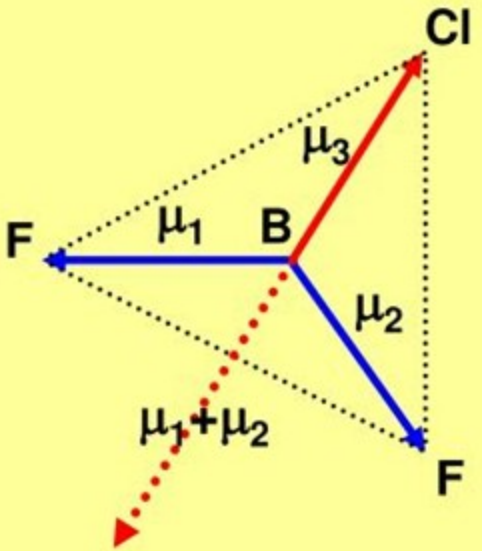


Different ligand atoms

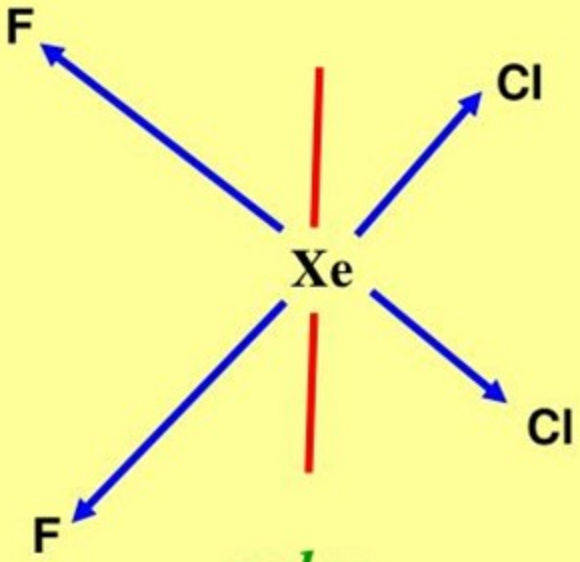
BF_2Cl

$|\mu_1+\mu_2| > |\mu_3|$

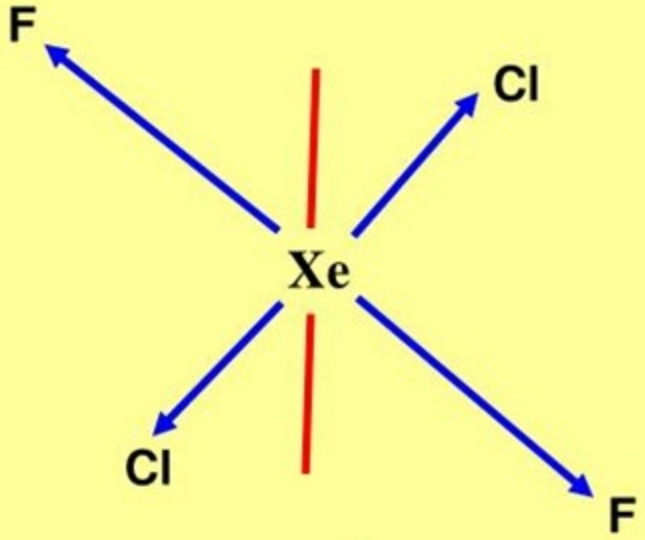
Net dipole moment ≠ 0



XeF_2Cl_2

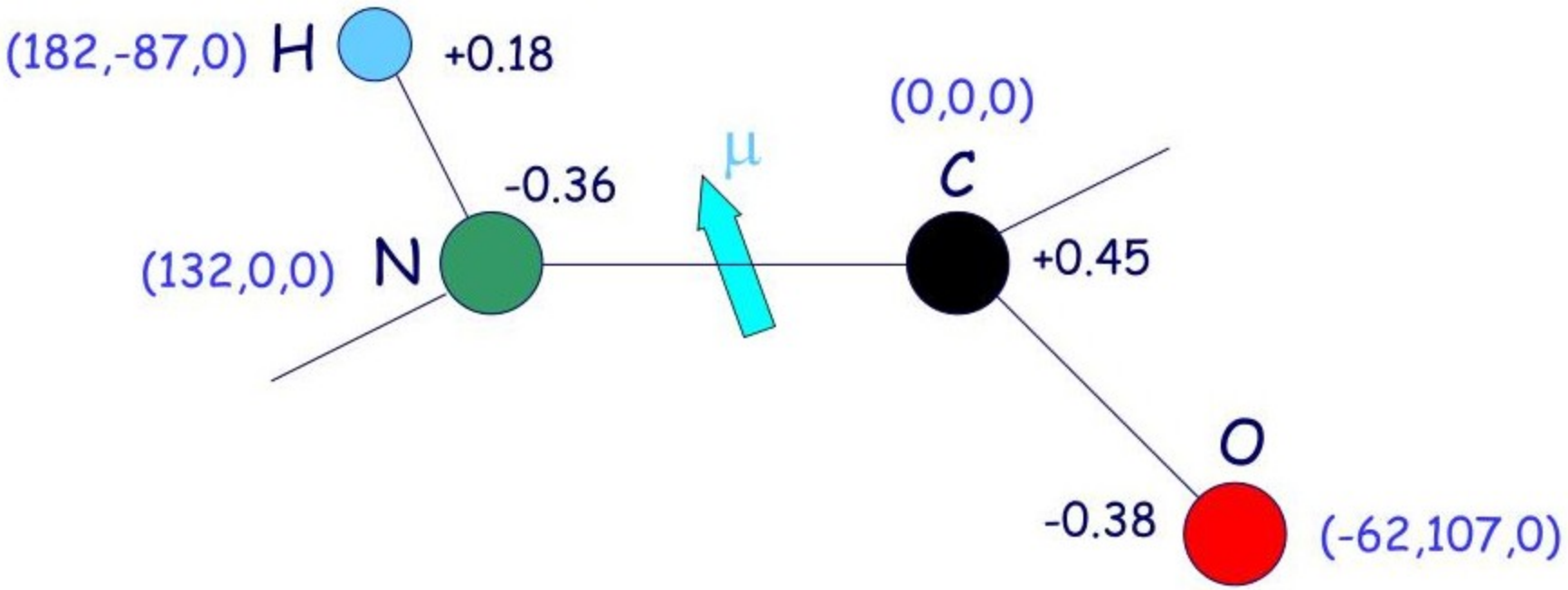


polar



nonpolar

Calculating a Molecular dipole moment



μ_x = (-0.36e) x (132 pm) + (0.45e) x (0 pm)
+(0.18e) x (182 pm) + (-0.38e) x (-62 pm)
= 8.8e pm
= 8.8 x (1.602×10^{-19} C) x (10^{-12} m)
= 1.4×10^{-30} C m = 0.42 D

Nonpolar

The dipole moments of two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.

Polar

The dipole moments of two polar bonds with an angle of less than 180° between them will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

Nonpolar

The dipole moments of three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.

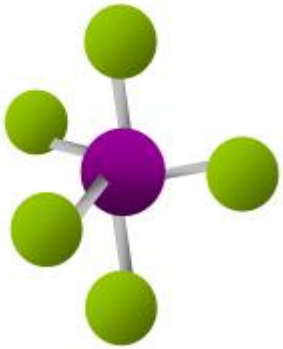
Nonpolar

The dipole moments of four identical polar bonds in a tetrahedral arrangement (109.5° from each other) will cancel. The molecule is nonpolar.

Polar

The dipole moments of three polar bonds in a trigonal pyramidal arrangement (109.5° from each other) will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

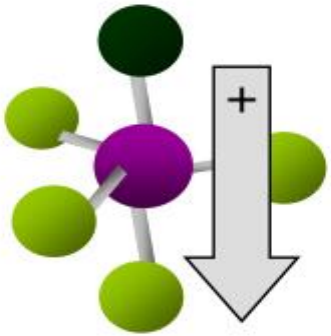
Molecular Geometry
Dipole Moment and Polarity



PF_5

Non polar

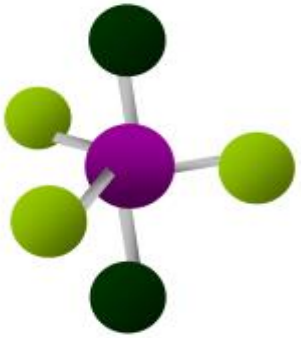
VSEPR shape
identical atoms



PF_4Cl

Polar

VSEPR
shape
atoms differ

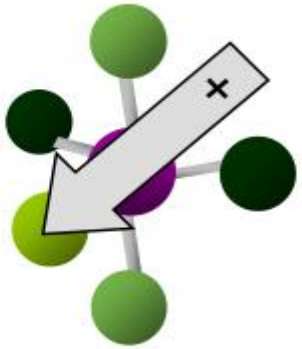


PF_3Cl_2

Non polar

Atoms differ. ***BUT*** can be divided into nonpolar VSEPR shapes:

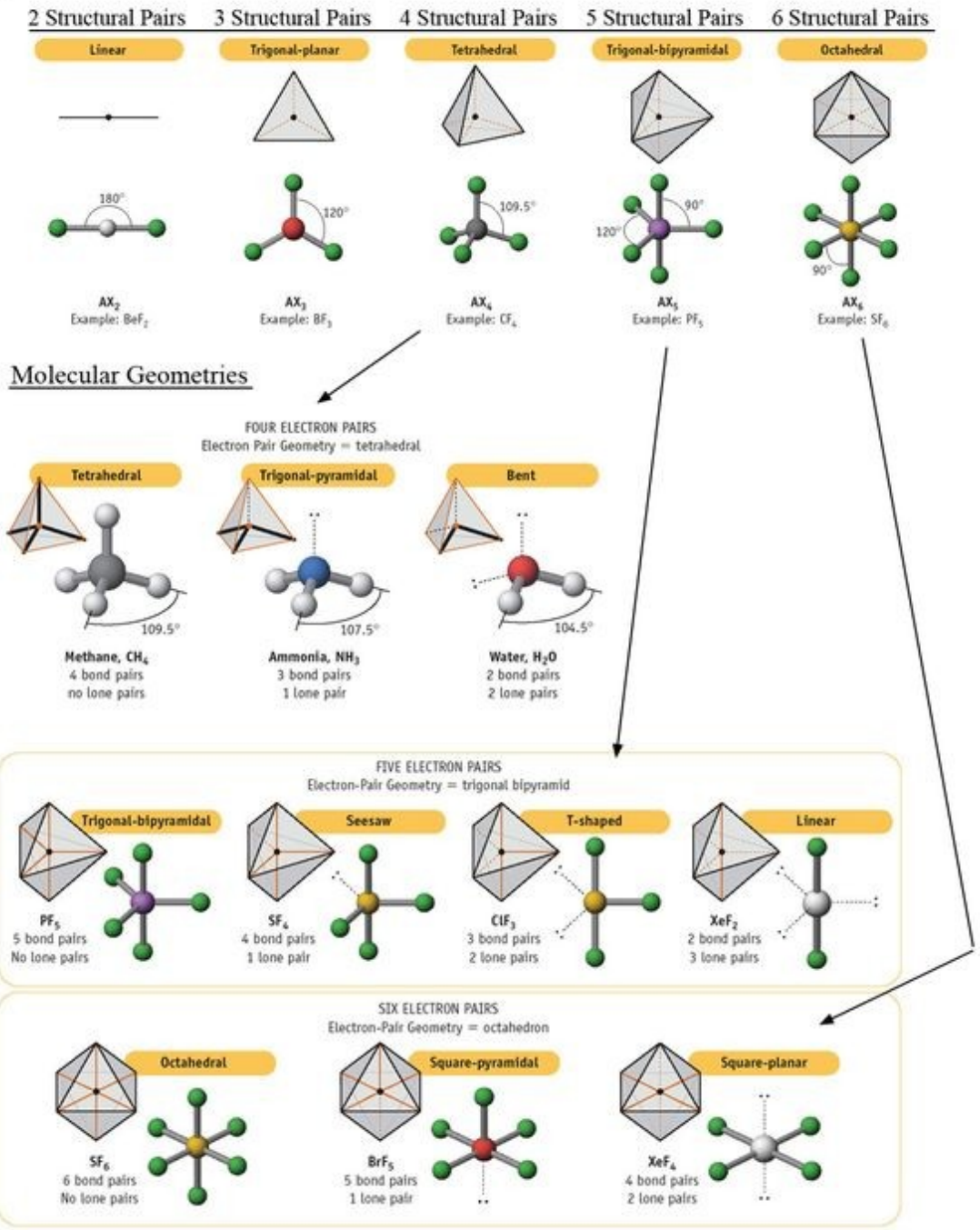
linear + triangular planar



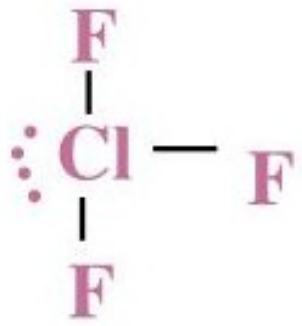
PF_3Cl_2

Polar

Atoms differ. Doesn't divide into nonpolar VSEPR shapes


Electron Pair Geometries
2 Structural Pairs
3 Structural Pairs
4 Structural Pairs
5 Structural Pairs
6 Structural Pairs
Linear
Trigonal-planar
Tetrahedral
Trigonal-bipyramidal
Octahedral
180°
120°
109.5°
120°
90°
90°
AX2
Example: BeF2
AX3
Example: BF3
AX4
Example: CF4
AX5
Example: PF5
AX6
Example: SF6
Molecular Geometries
FOUR ELECTRON PAIRS
Electron Pair Geometry = tetrahedral
Tetrahedral
Trigonal-pyramidal
Bent
109.5°
107.5°
104.5°
Methane, CH4
4 bond pairs
no lone pairs
Ammonia, NH3
3 bond pairs
1 lone pair
Water, H2O
2 bond pairs
2 lone pairs
FIVE ELECTRON PAIRS
Electron-Pair Geometry = trigonal bipyramid
Trigonal-bipyramidal
Seesaw
T-shaped
Linear
PF5
5 bond pairs
No lone pairs
SF4
4 bond pairs
1 lone pair
ClF3
3 bond pairs
2 lone pairs
XeF2
2 bond pairs
3 lone pairs
SIX ELECTRON PAIRS
Electron-Pair Geometry = octahedron
Octahedral
Square-pyramidal
Square-planar
SF6
6 bond pairs
No lone pairs
BrF5
5 bond pairs
1 lone pair
XeF4
4 bond pairs
2 lone pairs

Dipole Moment and Molecular Geometry



ClF_3

T-shaped
No symmetry → polar

SF_4

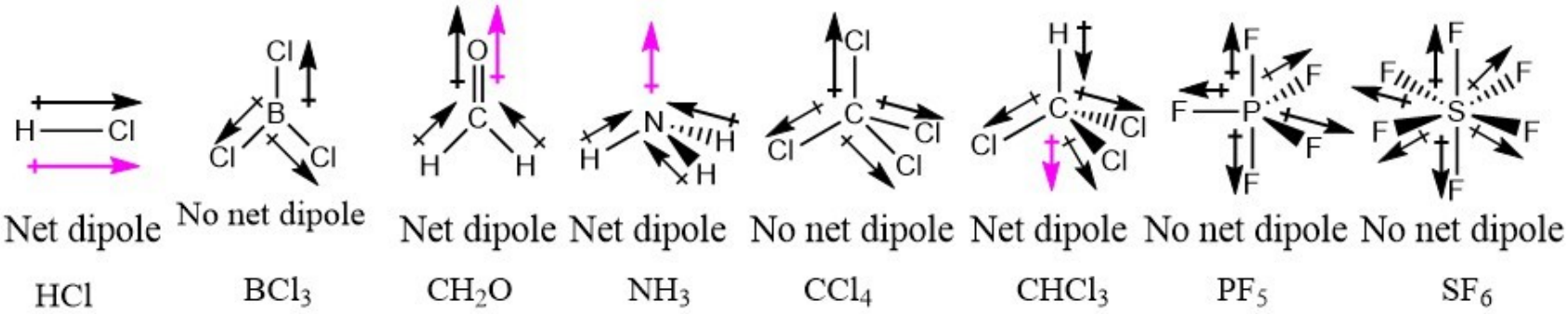
SeeSaw
No symmetry → polar

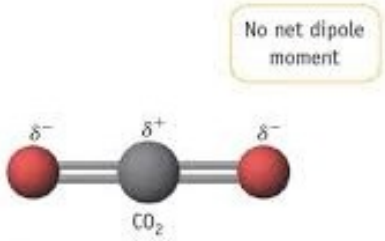
XeF_4

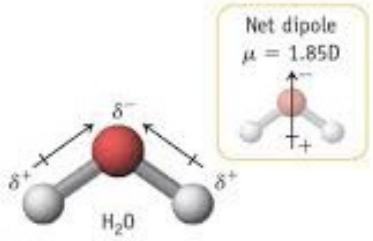
Square Planar
Symmetric → non polar

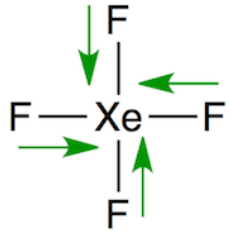
XeF_2

Linear
Symmetric → non polar

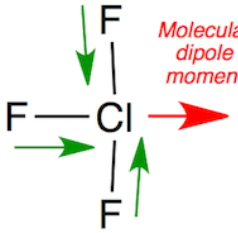




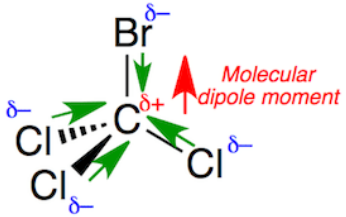




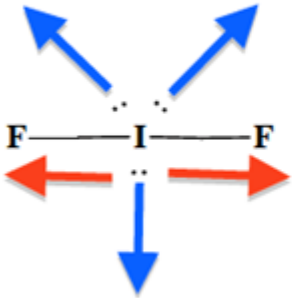
The four dipoles within the square planar molecule cancel each other out
XeF_4 is non-polar

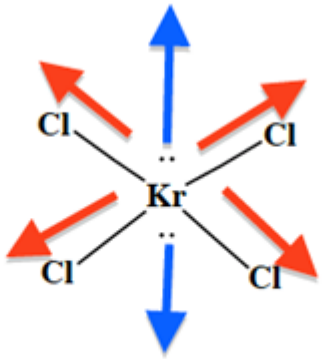


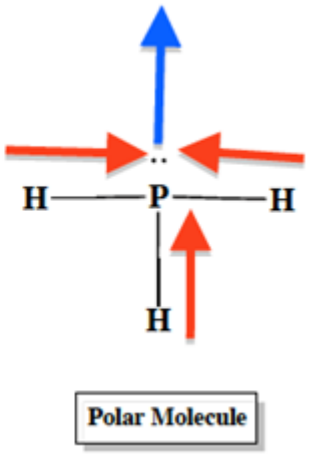
The three dipoles within the T-shaped molecule do not cancel each other out
ClF_3 is polar



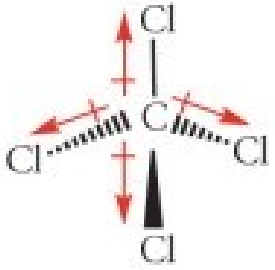
The C–Br bond is less polar than the C–Cl bonds
CCl_3Br has a small dipole



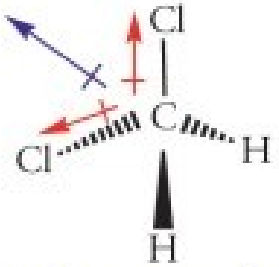




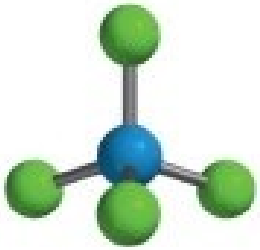
Blue arrow: direction of net dipole moment.



The bond moments cancel and there is no net polarity.

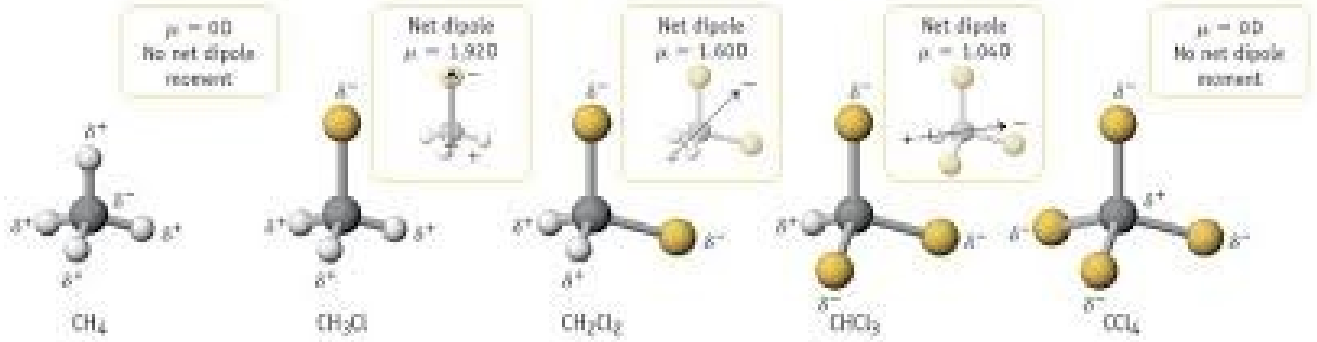


The bond moments do not cancel and there is a net polarity.



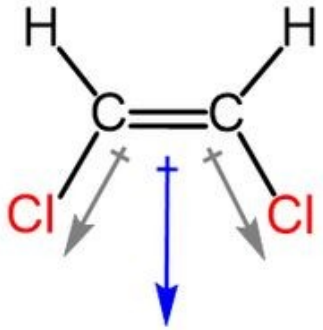
Tetrachloromethane

Dichloromethane



How the Molecular Dipole Moment Affects the Physical Properties

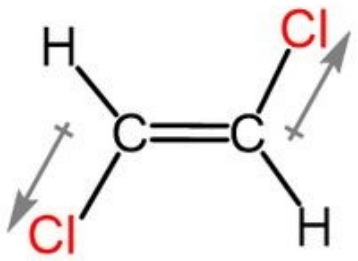
cis-1,2-Dichloroethene



net dipole moment

μ = 1.9 D

trans-1,2-Dichloroethene



Opposite dipoles cancel

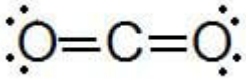
μ = 0 D

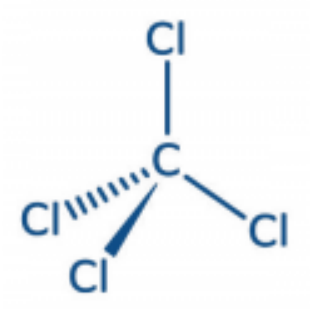
bp 60 °C *(higher)*	**vs**	**boiling point 48 °C**
melting point -80 °C	**vs**	**mp -50 °C *(higher)***

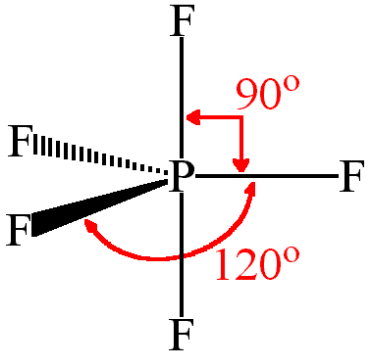
Intermolecular dipole-dipole interactions increase the b.p.

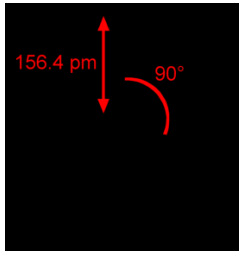
Symmetrical strucutres have higher melting point.

Proč jsou molekuly CO_2, BF_3, CCl_4, PF_5, SF_6 nepolární ?

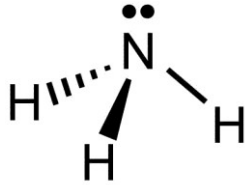








NH_3 je polární, ale BF_3 je nepolární. Proč?



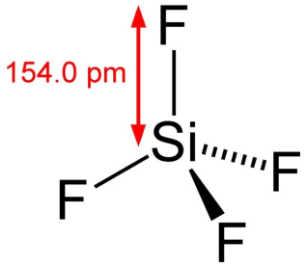
Která z těchto molekul je polární ?

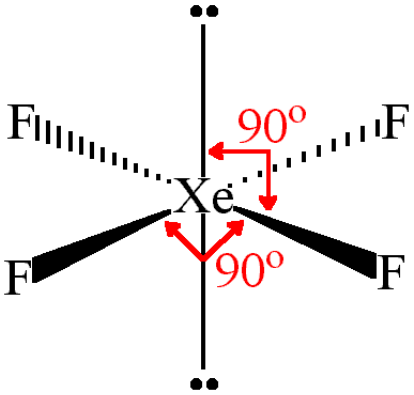
(a) SiF_4

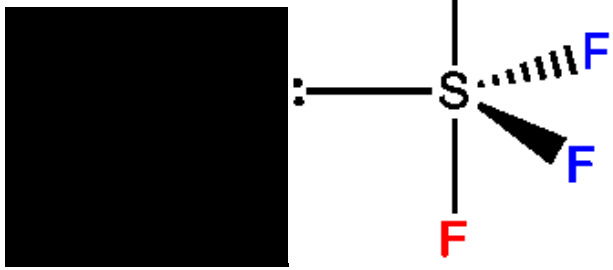
(b) XeF_4

(c) BF_3

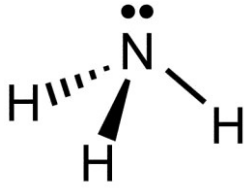
(d) SF_4

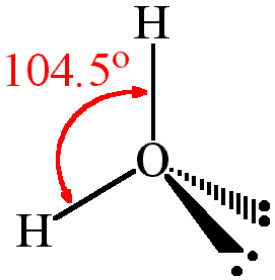




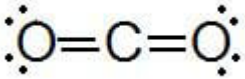


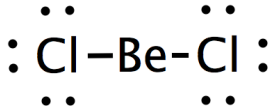
Která z molekul BF_3, NH_3 a H_2O má nulový dipólový moment ?

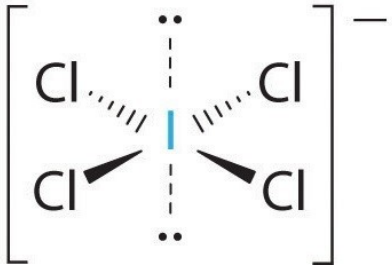


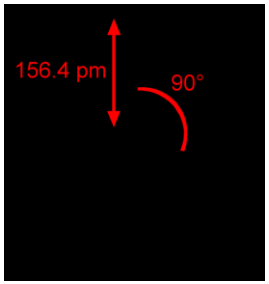


Která z molekul CO_2, $BeCl_2$, ICl_4^- a SF_6 má nulový dipólový moment ?









Proč má molekula BeH_2 nulový dipól, přestože je vazba Be-H polární ?

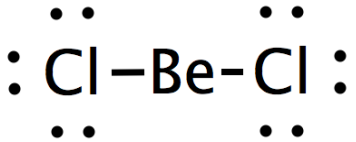
Molekula H_2O má nenulový dipólový moment a molekula BeF_2 má nulový dipólový moment protože

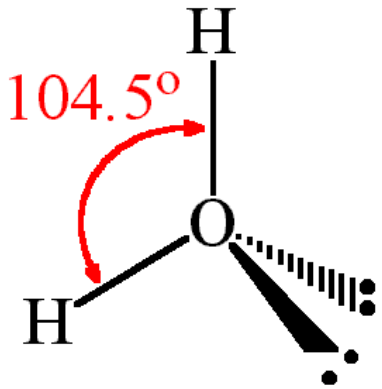
(a) molekula H_2O má lineární tvar, zatímco molekula BeF_2 je lomená.

(b) molekula BeF2 má lineární tvar, zatímco molekula H_2O je lomená.

(c) fluor má vyšší elektronegativitu než kyslík.

(d) beryllium má vyšší elektronegativitu než kyslík.





Dipólový moment molekuly CO_2 je nulový, zatímco u molekuly SO_2 je dipólový moment nenulový. Proč?