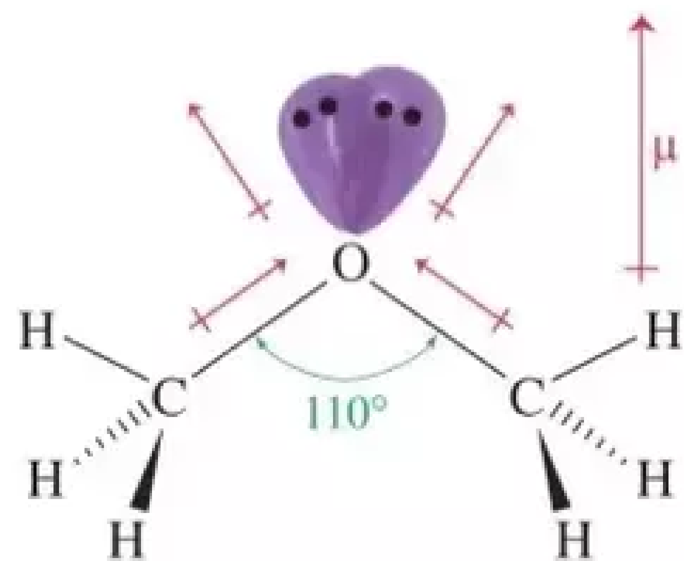
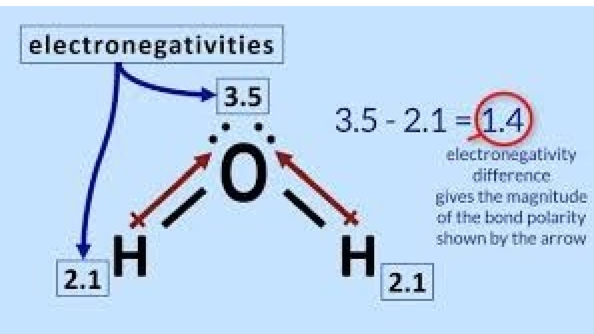
Structure and Polarity

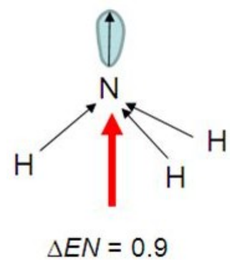
- Oxygen is sp^3 hybridized.
- Bent molecular geometry.
- C—O—C angles is 110°.
- Polar C—O bonds.
- Dipole moment of 1.3 D.

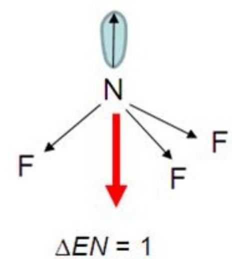


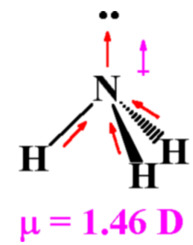
Polarita molekuly, dipólový moment

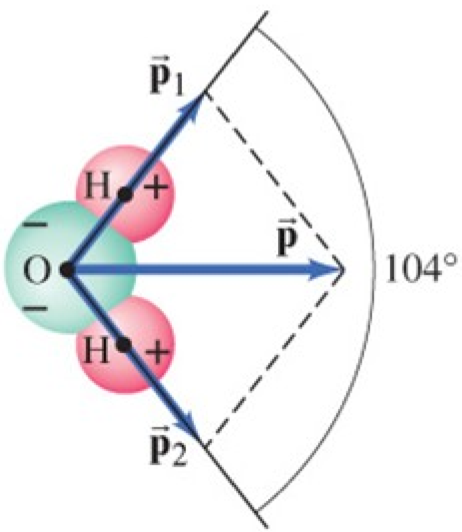
Dipolový moment molekuly = vektorový součet všech vazebných dipolů. Může být nulový, i v případě nenulových vazebných dipolů které se navzájem kompenzují (např. SF_6, SiF_4, CF_4, …)

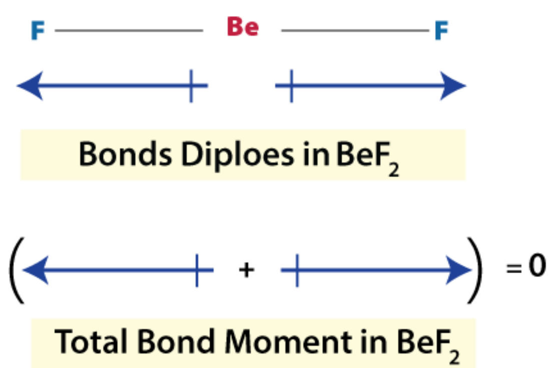


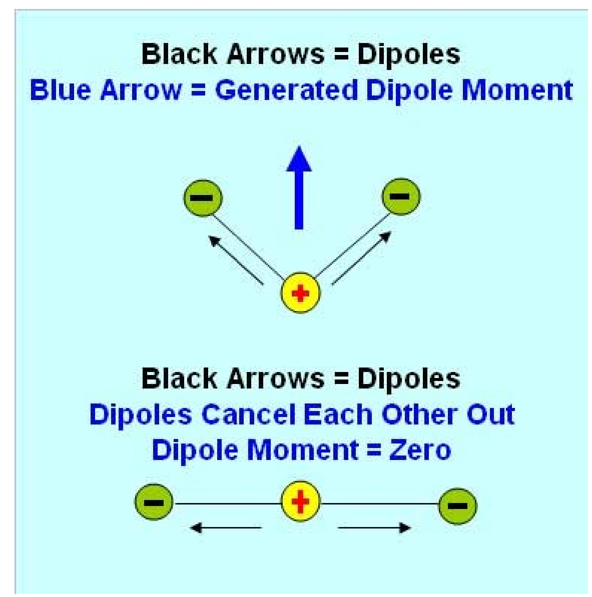










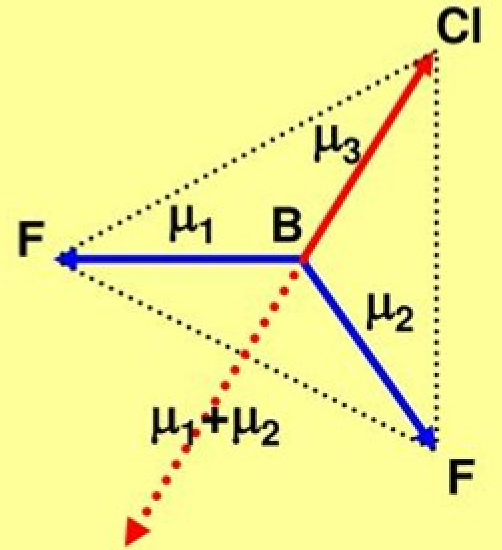


Different ligand atoms

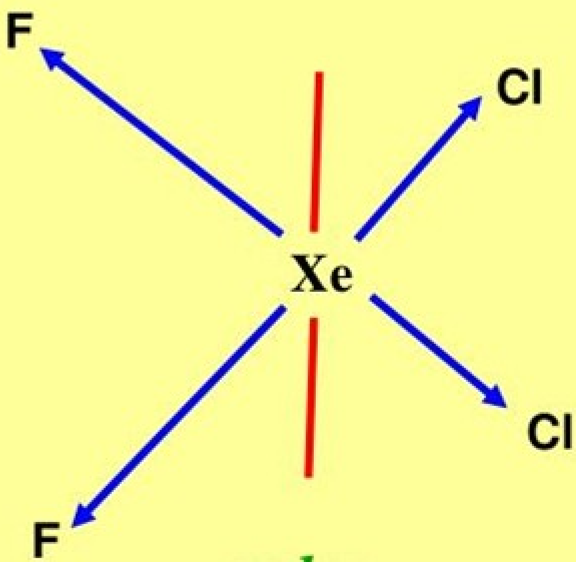
BF_2Cl

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

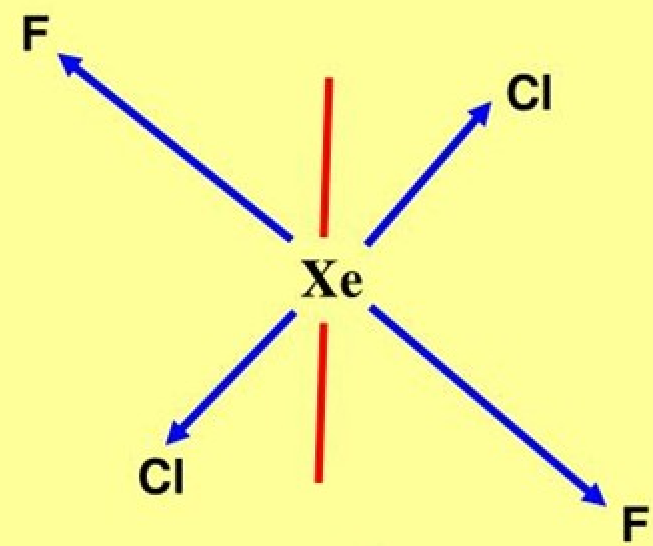
Net dipole moment ≠ 0



XeF_2Cl_2

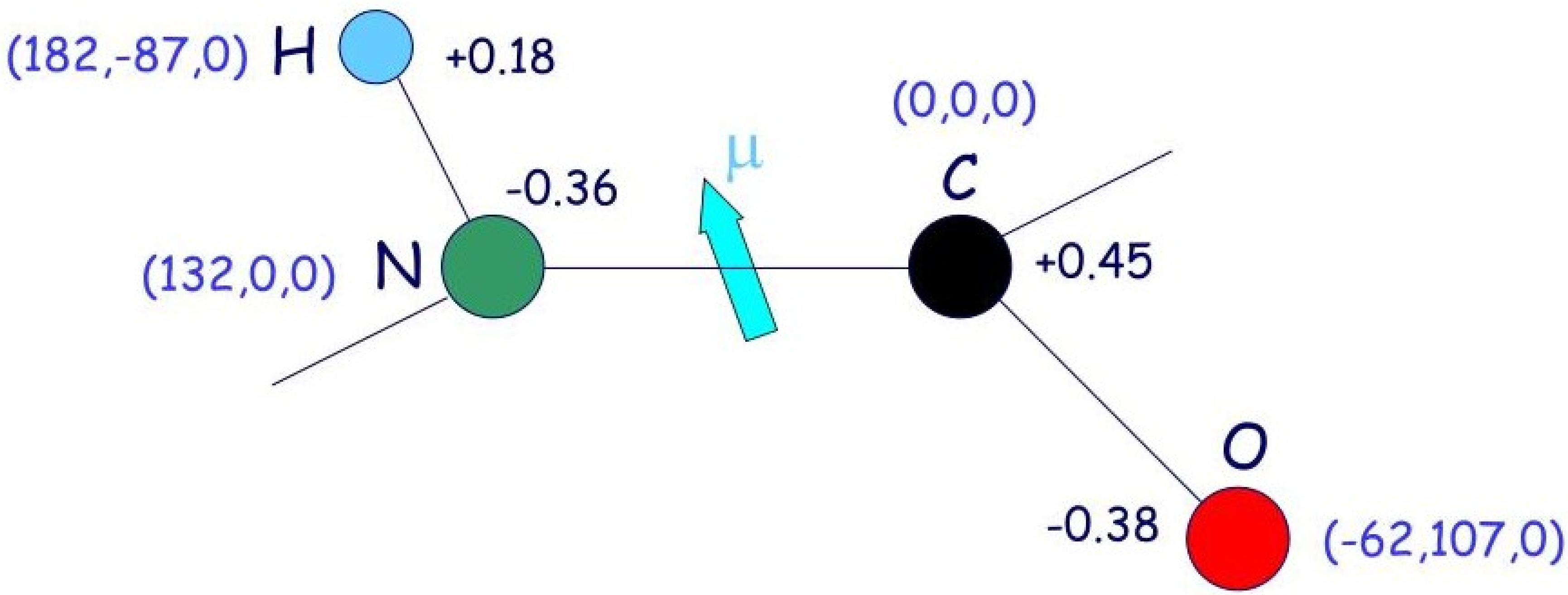


polar



nonpolar

Calculating a Molecular dipole moment



$$\mu_x = (-0.36e) \times (132\ \text{pm}) + (0.45e) \times (0\ \text{pm}) + (0.18e) \times (182\ \text{pm}) + (-0.38e) \times (-62\ \text{pm})$$

$$= 8.8e\ \text{pm}$$

$$= 8.8 \times (1.602 \times 10^{-19}\ C) \times (10^{-12}\ \text{m})$$

$$= 1.4 \times 10^{-30}\ C\ \text{m} = 0.42\ \text{D}$$

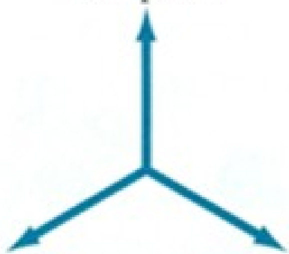
Nonpolar

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

Polar

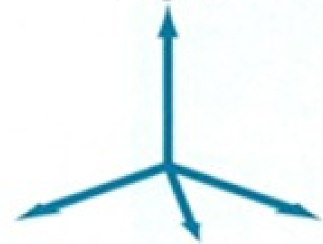
The dipole moments of two polar bonds with an angle of less than 180° between them will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

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.

TABLE 10.3 Common Cases of Adding Dipole Moments to Determine Whether a Molecule Is Polar

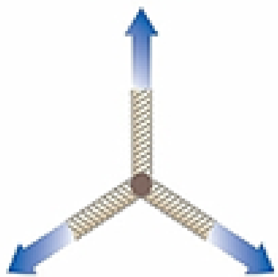
Nonpolar

Two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.

Polar

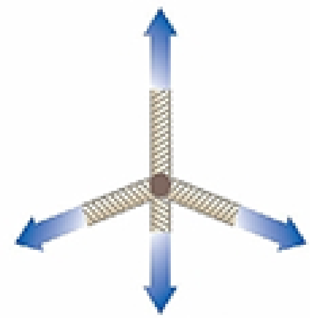
Two polar bonds with an angle of less than 180° between them will not cancel. The molecule is polar.

Nonpolar



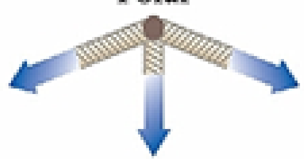
Three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.

Nonpolar



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

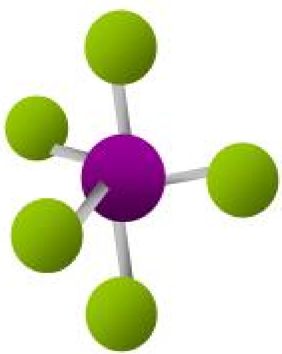
Polar



Three polar bonds in a trigonal pyramidal arrangement (109.5°) will not cancel. The molecule is polar.

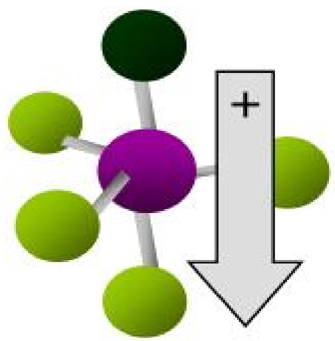
Note: In all cases where the polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different than the other(s), the bonds will not cancel and the molecule is polar.

Molecular Geometry
Dipole Moment and Polarity



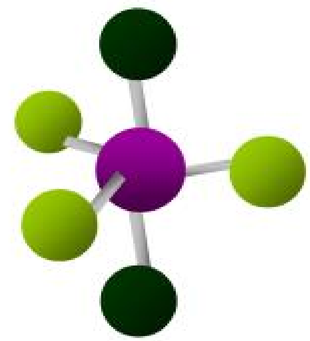
PF_5

Non polar
VSEPR shape
identical atoms



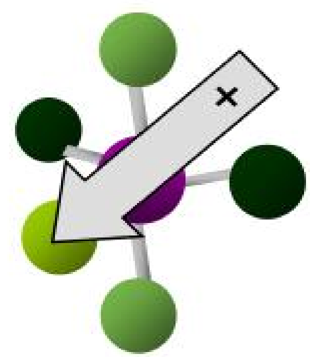
PF_4Cl

Polar
VSEPR
shape
atoms differ



PF_3Cl_2

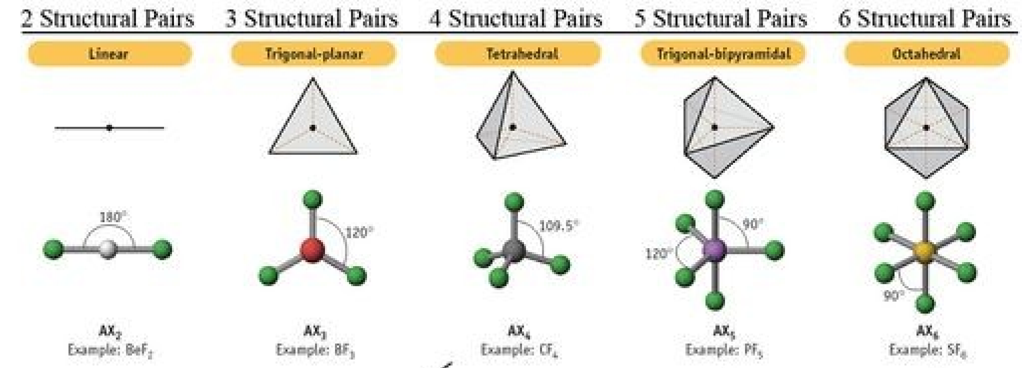
Non polar
Atoms differ. ***BUT*** can be divided into nonpolar VSEPR shapes:
linear + triangular planar



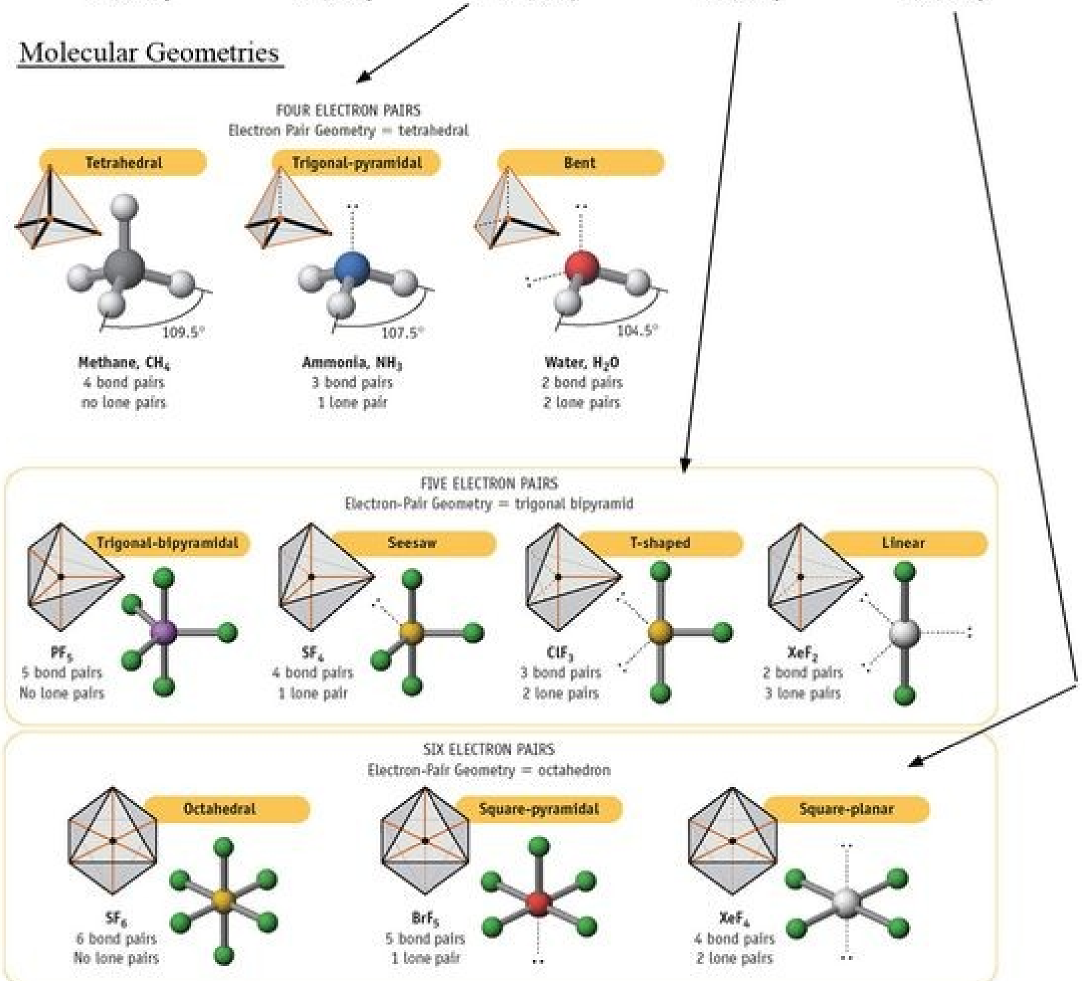
PF_3Cl_2

Polar
Atoms differ. Doesn't divide into nonpolar VSEPR shapes

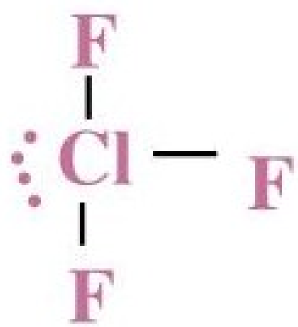
Electron Pair Geometries



Molecular Geometries



Dipole Moment and Molecular Geometry



ClF_3

T-shaped
No symmetry → polar

SF_4

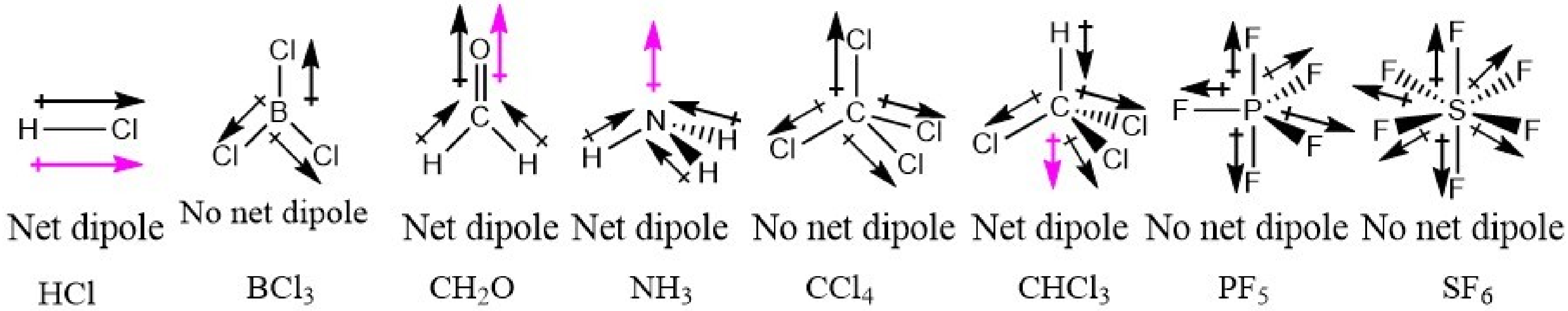
SeeSaw
No symmetry → polar

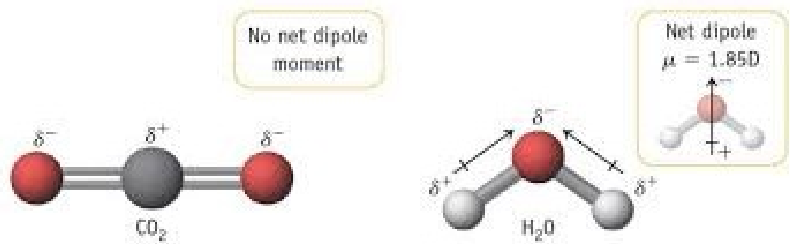
XeF_4

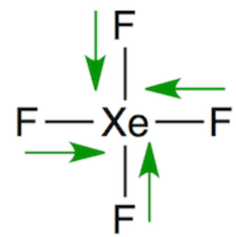
Square Planar
Symmetric → non polar

XeF_2

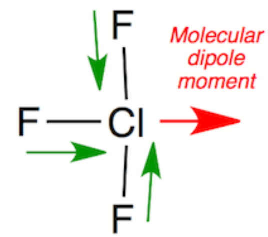
Linear
Symmetric → non polar



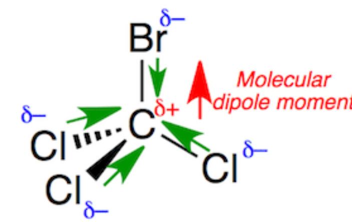




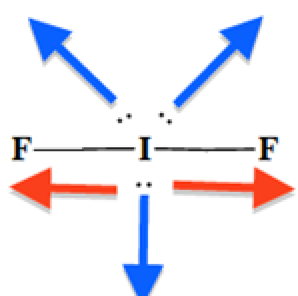
The four dipoles within the square planar molecule cancel each other out
XeF_4 is non-polar



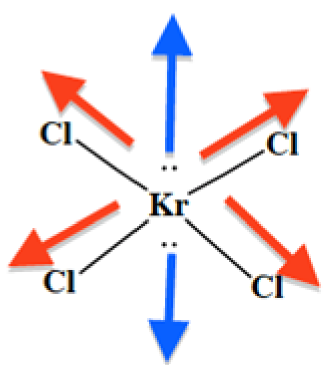
The three dipoles within the T-shaped molecule do not cancel each other out
ClF_3 is polar



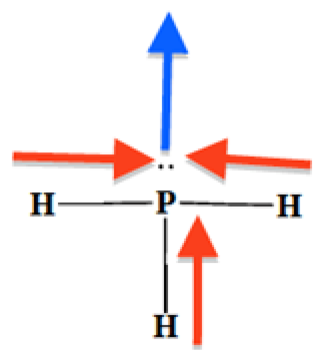
The C–Br bond is less polar than the C–Cl bonds
CCl_3Br has a small dipole



Nonpolar Molecule

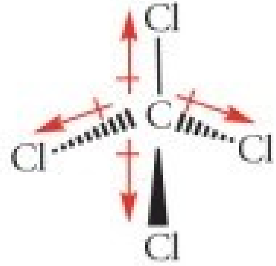


Nonpolar Molecule

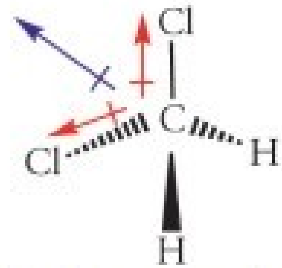


Polar Molecule

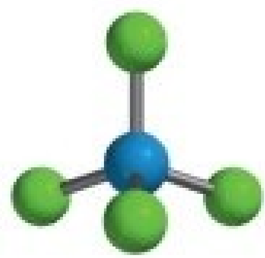
Blue arrow: direction of net dipole moment.



The bond moments cancel and there is no net polarity.

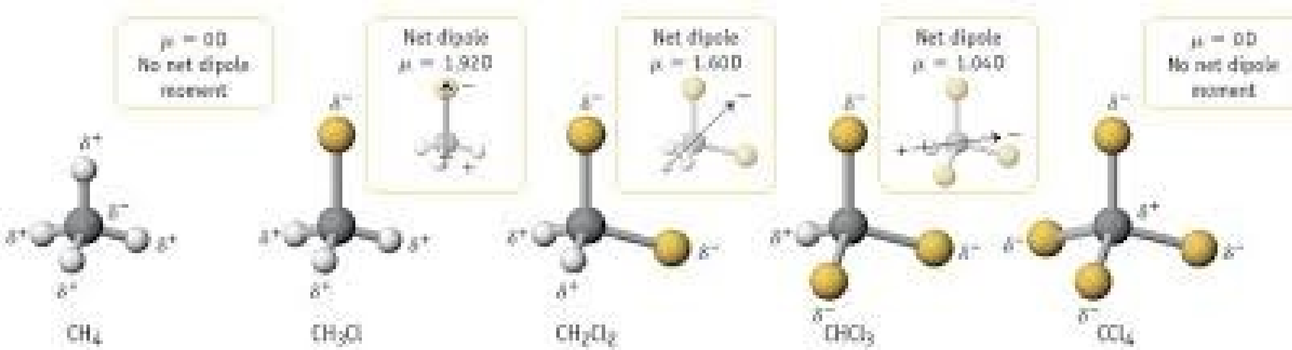


The bond moments do not cancel and there is a net polarity.



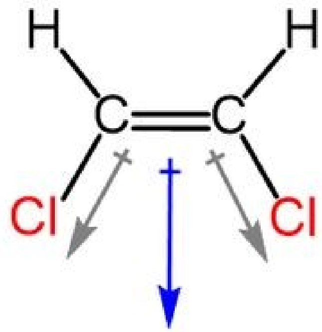
Tetrachloromethane

Dichloromethane



How the Molecular Dipole Moment Affects the Physical Properties

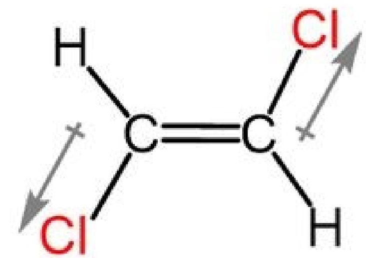
cis-1,2-Dichloroethene



net dipole moment

μ = 1.9 D

trans-1,2-Dichloroethene



Opposite dipoles cancel

μ = 0 D

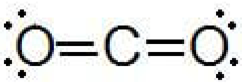
bp 60 ^{o}C ***(higher)*** **vs** **boiling point 48 ^{o}C**

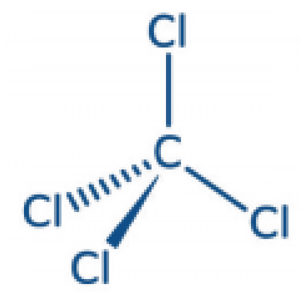
melting point -80 ^{o}C **vs** **mp -50 ^{o}C** ***(higher)***

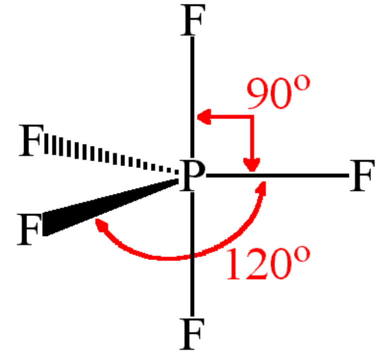
Intermolecular dipole-dipole interactions increase the b.p.

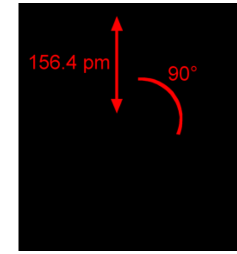
Symmetrical strucutres have higher melting point.

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

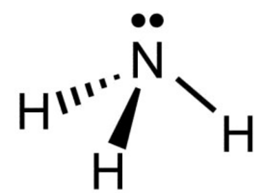








NH_3 je polární, ale BF_3 je nepolární. Proč?



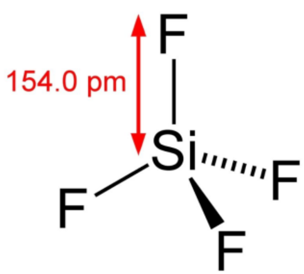
Která z těchto molekul je polární ?

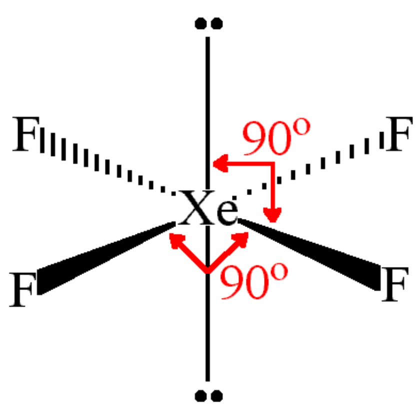
(a) SiF_4

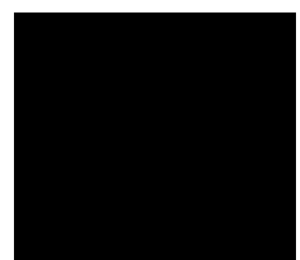
(b) XeF_4

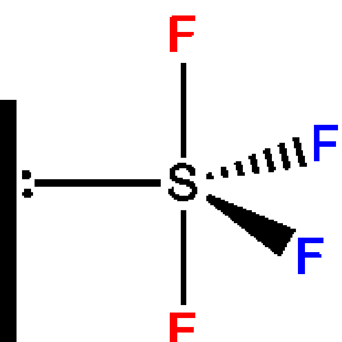
(c) BF_3

(d) SF_4

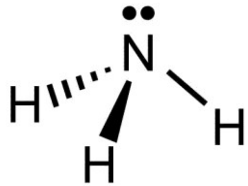


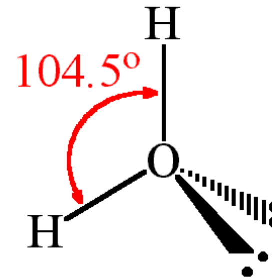




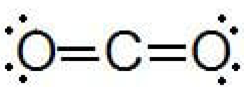


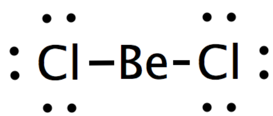
Která z molekul BF_3, NH_3 a H_2O má nulový dipólový moment ?

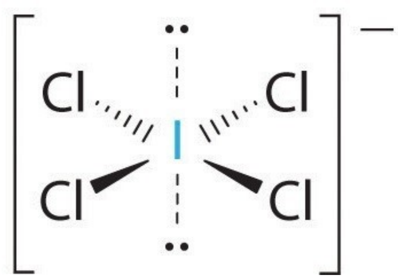


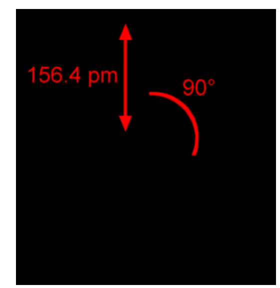


Která z molekul CO_2, $BeCl_2$, ICl_4^- a SF_6 má nulový dipólový moment ?





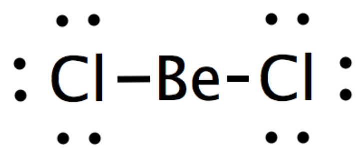


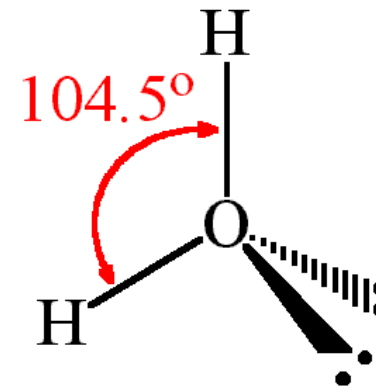


Proč má molekula BeH_2 nulový dipól, přestože je vazba Be-H polární ?

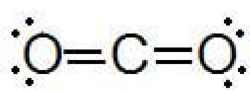
Molekula H_2O má nenulový dipólový moment a molekula BeF_2 má nulový dipólový moment protože

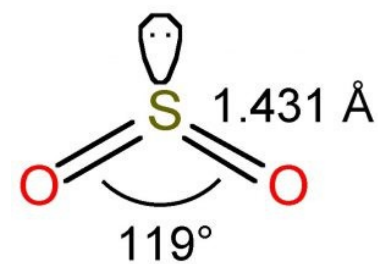
(a) molekula H_2O má lineární tvar, zatímco molekula BeF_2 je lomená.
(b) molekula BeF_2 má lineární tvar, zatímco molekula H_2O je lomená.
(c) fluor má vyšší elektronegativitu než kyslík.
(d) beryllium má vyšší elektronegativitu než kyslík.





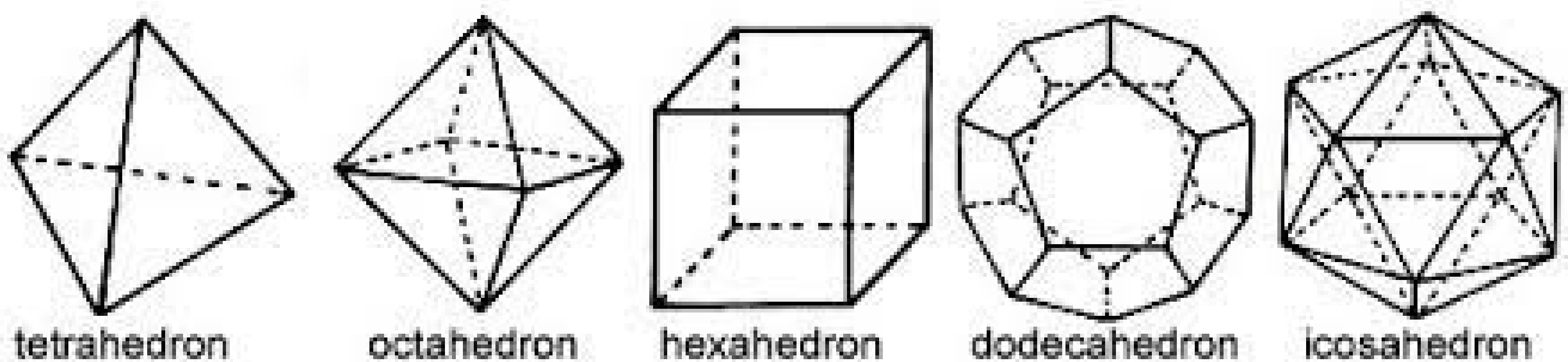
Dipólový moment molekuly CO_2 je nulový, zatímco u molekuly SO_2 je dipólový moment nenulový. Proč?

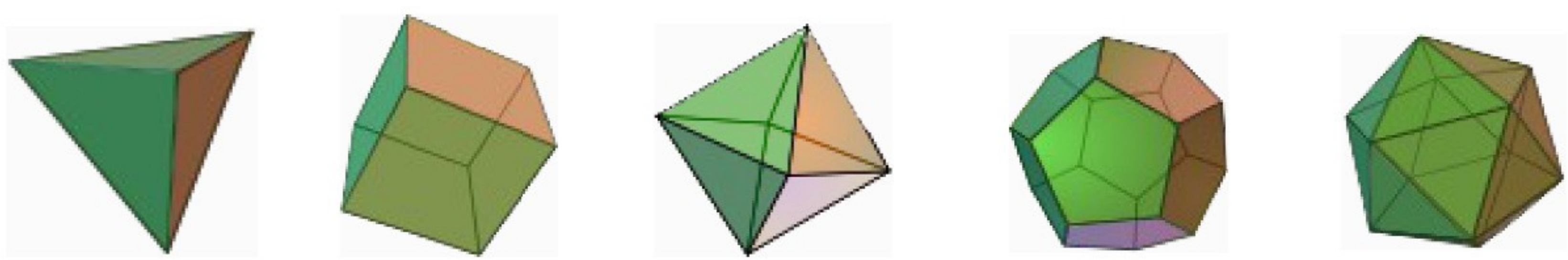




Platónská tělesa

Pravidelný mnohostěn je těleso, jehož stěny jsou tvořeny pravidelnými mnohoúhelníky, jichž se v každém vrcholu stýká stejný počet. Pravidelné mnohostěny nazýváme **platónská tělesa**.

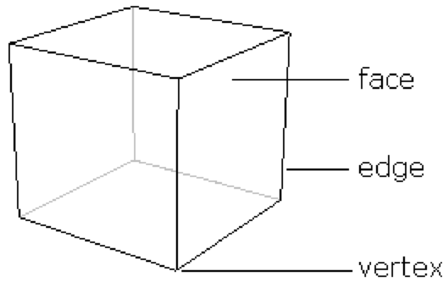




čtyřstěn *šestistěn* *osmistěn* *dvanáctistěn* *dvacetistěn*

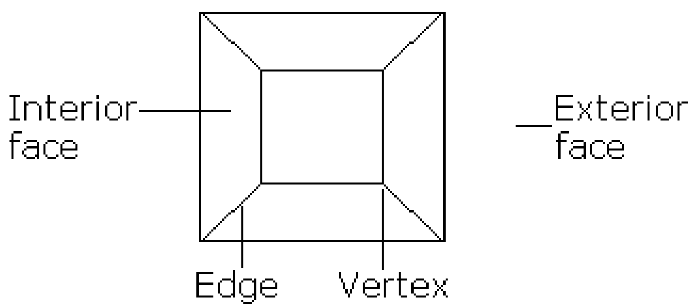
Eulerův vzorec

Transformace do planárního grafu (Schlegelův diagram)



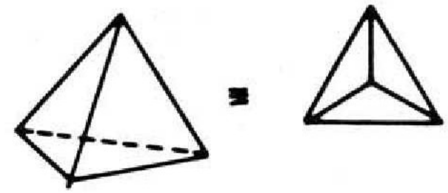
$$V - E + F = 2$$

V = počet vrcholů (vertices)
E = počet hran (edges)
F = počet ploch (faces)

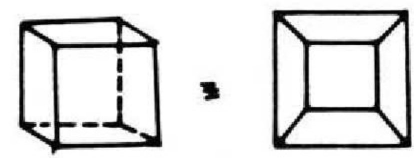


$$v - e + f = 1$$

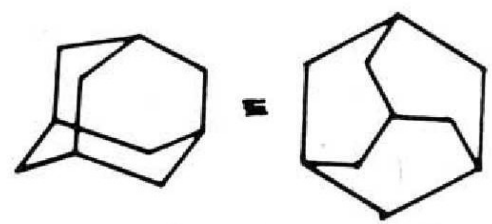
v = počet vrcholů (vertices)
e = počet hran (edges)
f = počet ploch (faces)



Tetrahedrane (a = 4, b = 6, c = 3) is tricyclo[1.1.0.0^{2,4}]butane.



Cubane (a = 8, b = 12, c = 5) is pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane.



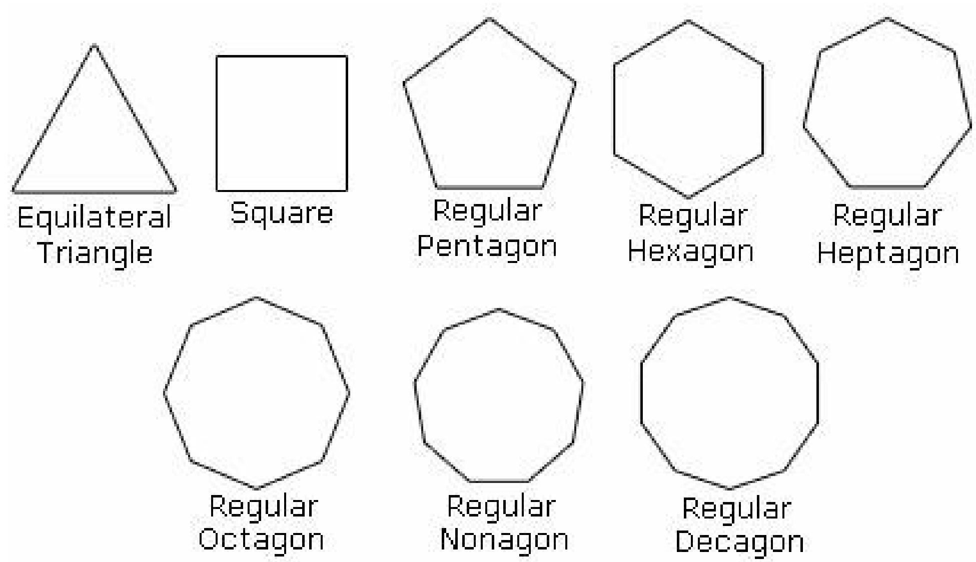
Adamantane (a = 10, b = 12, c = 3) is tricyclo[3.3.1.1^{3,7}]decane.

Lederberg J.: PNAS 53, 1965, 134-139
Eckroth D.R.: J. Org. Chem. 32, 1967, 3362-3365

Cyklické a nenasycené uhlovodíky

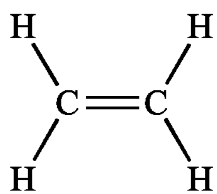
$$v - e + f = 1$$

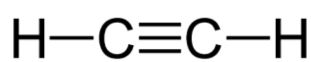
v = počet vrcholů (vertices)
e = počet hran (edges)
f = počet ploch (faces)

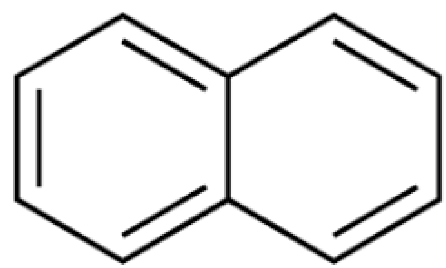


$$f = e - v + 1$$

f = tzv. cyklomatické číslo (počet cyklů a násobných vazeb v molekule)

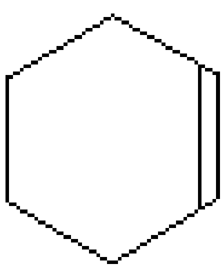




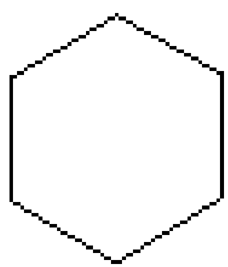


v = 10
e = 16
f = 7

naftalen



cyclohexene



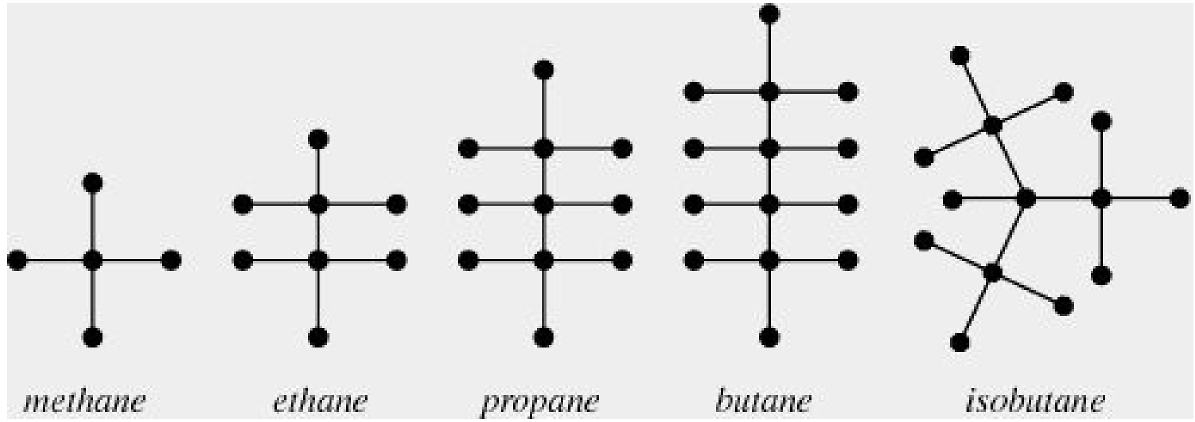
cyclohexane

Anantha Reddy P. : J. Chem. Educ. 64, 1987, 400.
Rouvray D.H.: J. Chem. Educ. 52, 1975, 768-773.

Alifatické alkany

$$v - e + 0 = 1$$

$$v = e - 1$$

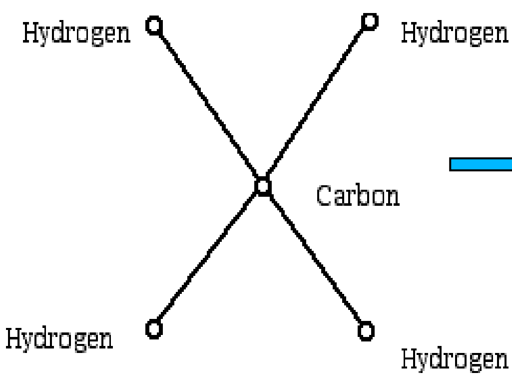


v = počet vrcholů (verices)
e = počet hran (edges)
f = počet ploch (faces) = 0

Stupeň vrcholu grafu (valence vrcholu) = počet hran zasahujících do daného vrcholu

$$\deg(v_1) + \deg(v_2) + \ldots + \deg(v_p) = 2(v - 1)$$

deg(C) = 4
deg(H) = 1



$$1 + 1 + 1 + 1 + 4 = 2(4 + 1 - 1)$$

$$h + 4c = 2(c + h - 1)$$

$$\mathbf{h = 2c + 2}$$

Gutman I. : Teach. Math. 11, 2008, 53-61.