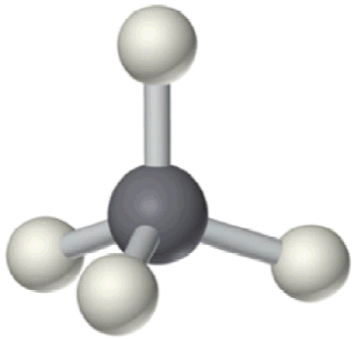
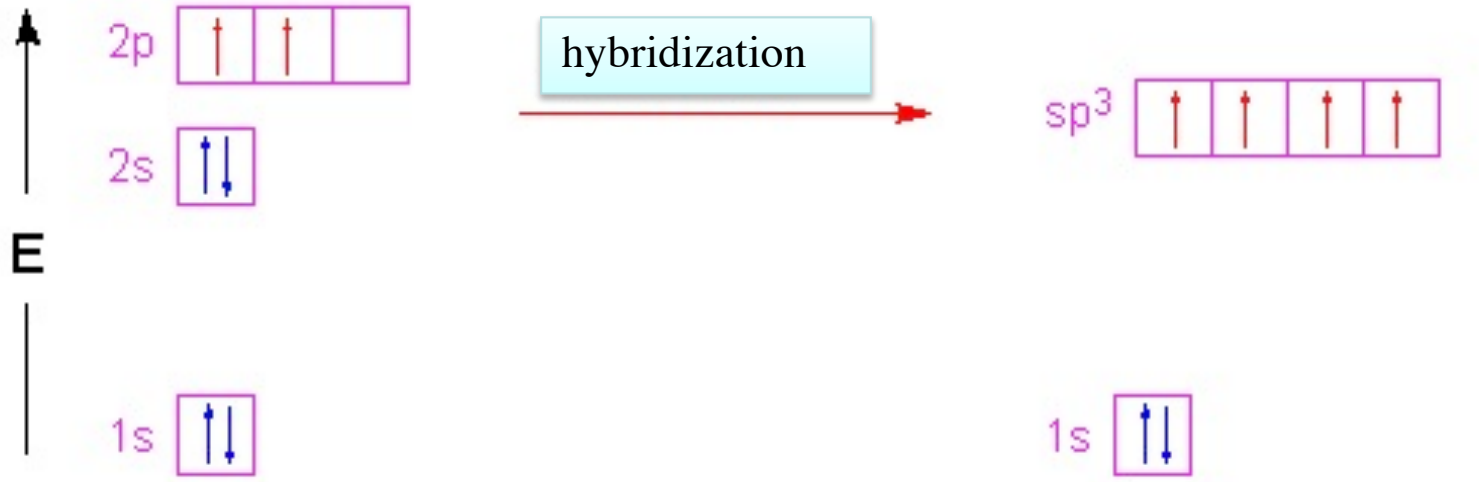
The shape of orbitals and hybrid orbitals.

If the four methane hydrogen atoms were bound by 3 p orbitals and 1 orbital s, the geometry would be: 90° , 90° , 90° , 135° .
The VESPR model (valence electron-shell pair repulsion) states that in order to maximize the distance between e^-, orbitals recombine with a new geometry to reach an energy minimum.

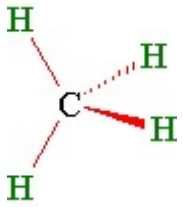


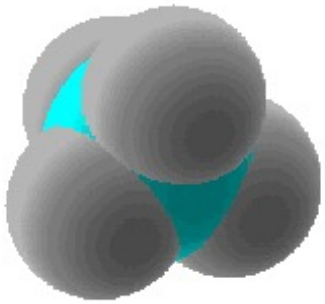
Methane, CH_4

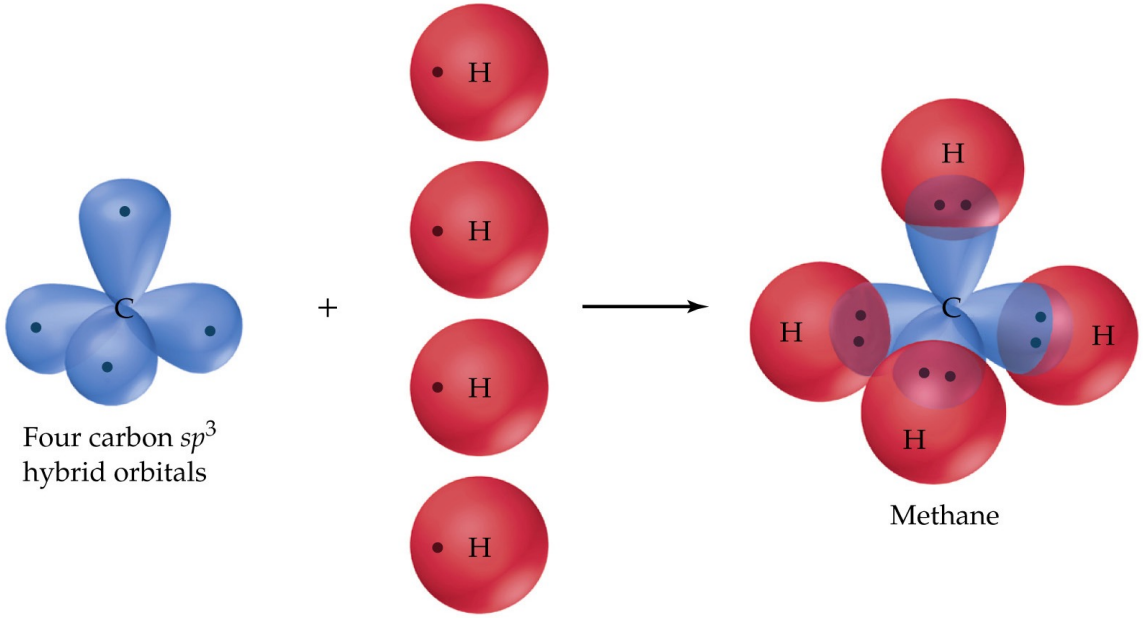
Recombination of 1 s orbital and 3 p orbitals: sp^3



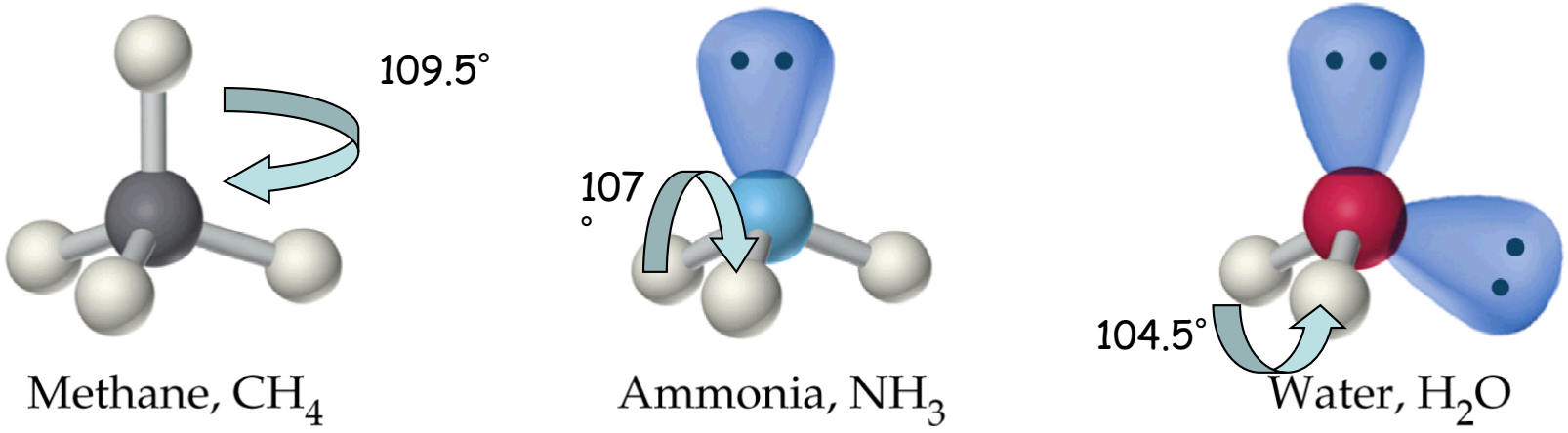
4 isoenergetic orbitals with tetrahedral geometry



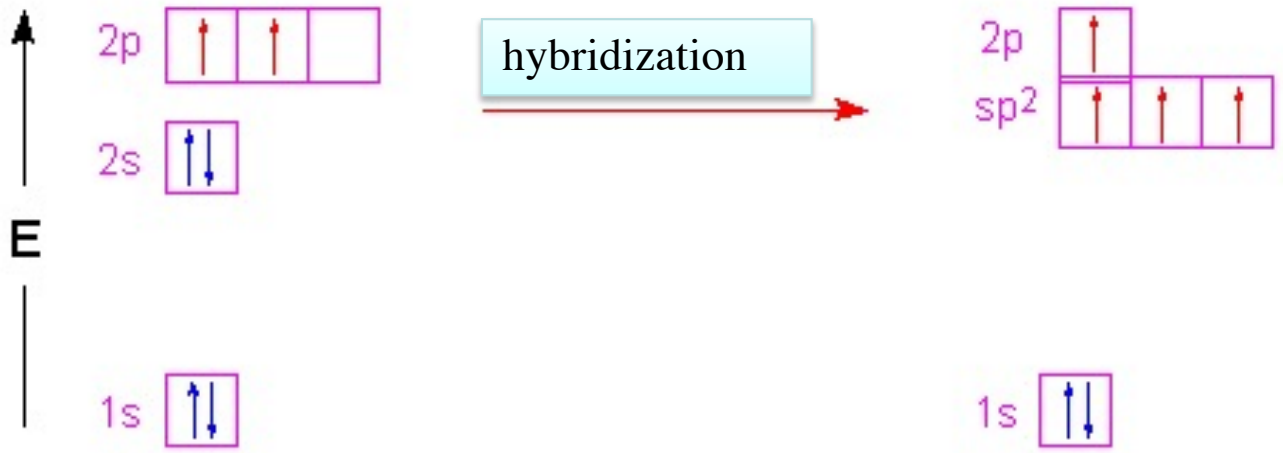




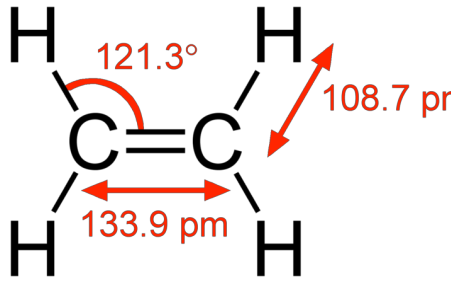
Orbitals that contain a lone pair induce a distortion and are available for coordiantion.

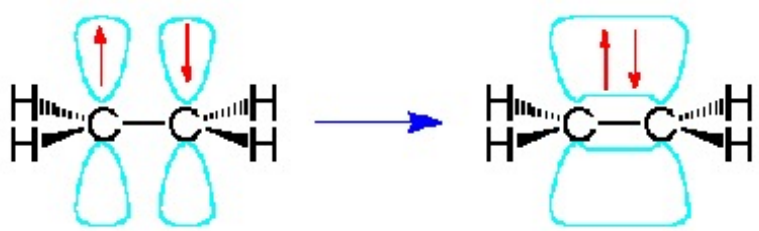


Recombination of 1 s orbital and 2 p orbitals: sp^2

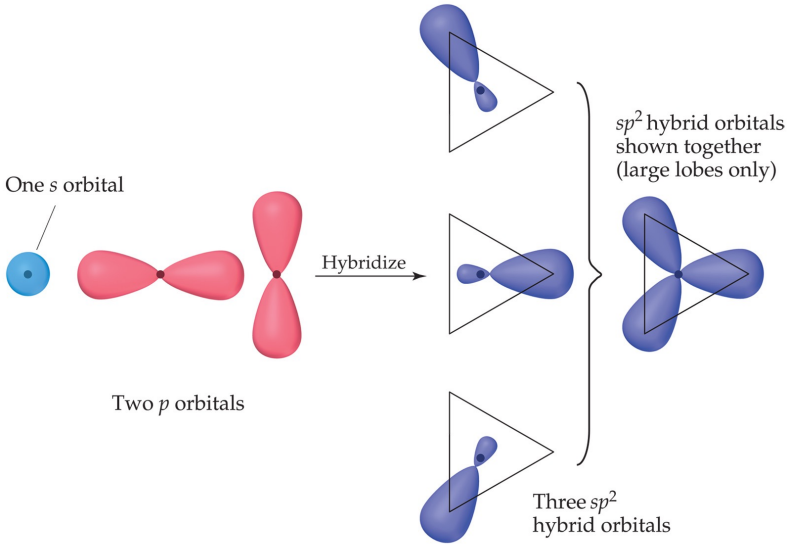


3 isoenergetic orbitals with trigonal geometry
+ 1 p orbital.

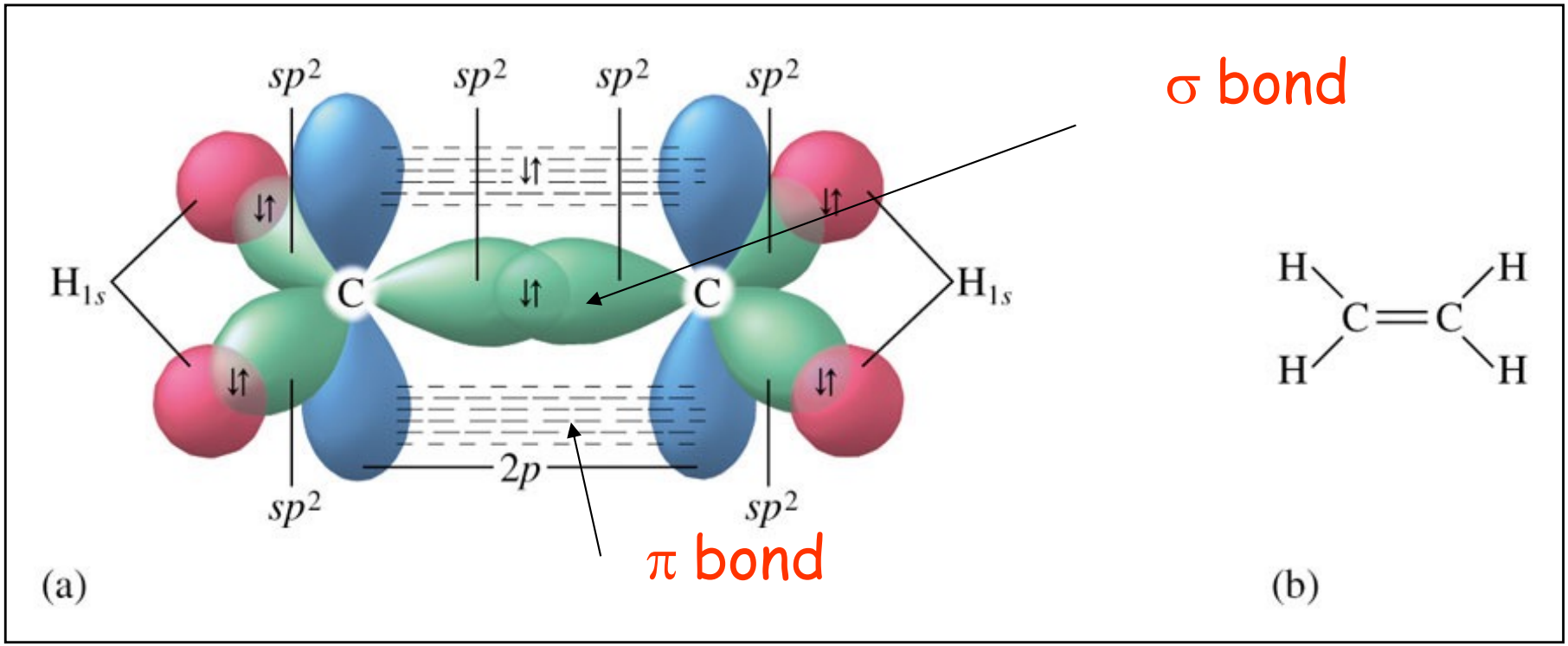




Example: ethene
(ethylene)

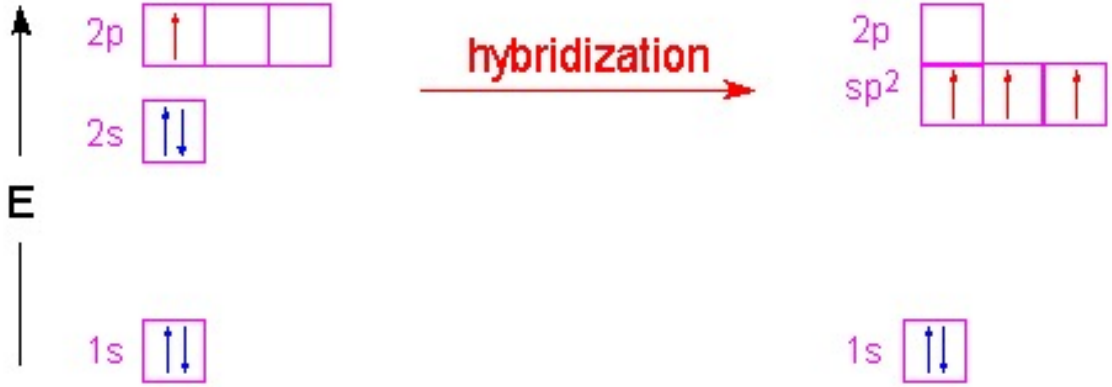


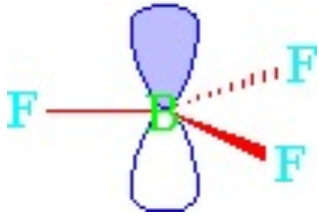
Sp^2: planar trigonal geometry (120°)



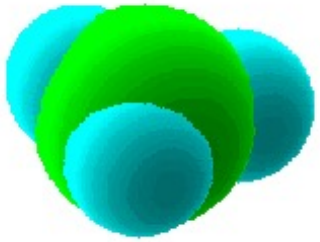
Double bonds can not rotate.

In BF_3 exception to the octet rule:

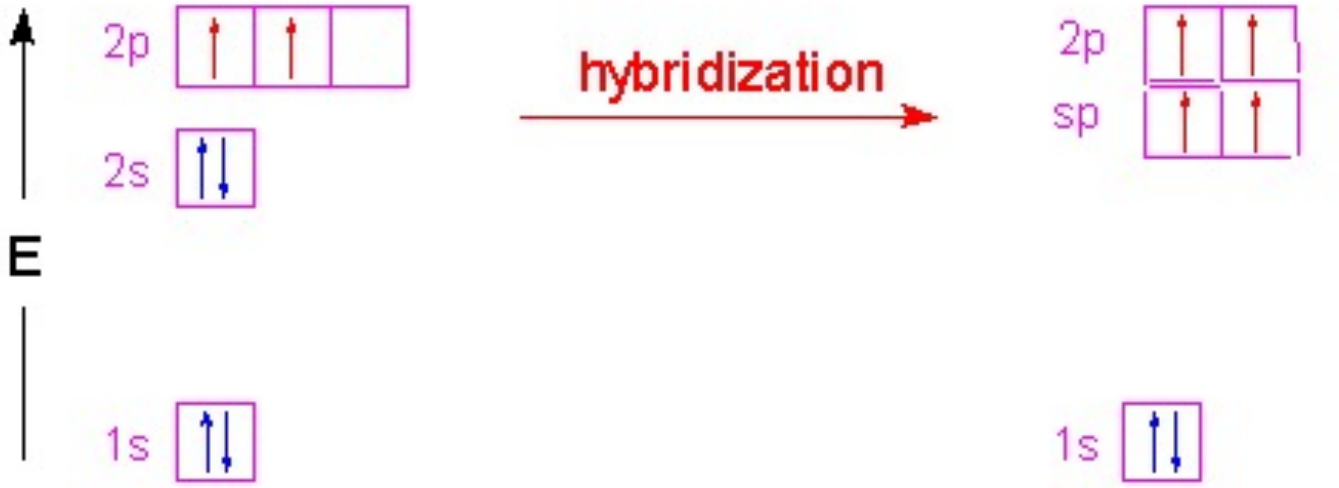




Empty p orbital + 3 sp^2 orbitals.



Recombination of 1 s orbital and 1 p orbital: sp



2 isoenergetic orbitals with linear geometry + 2 p orbitals.

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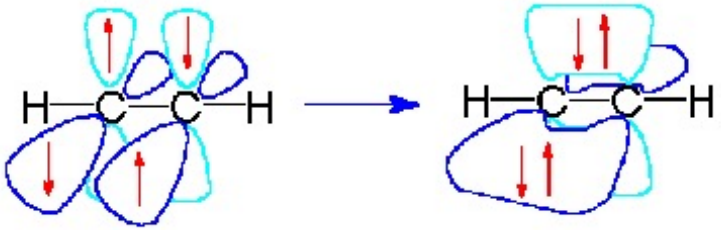
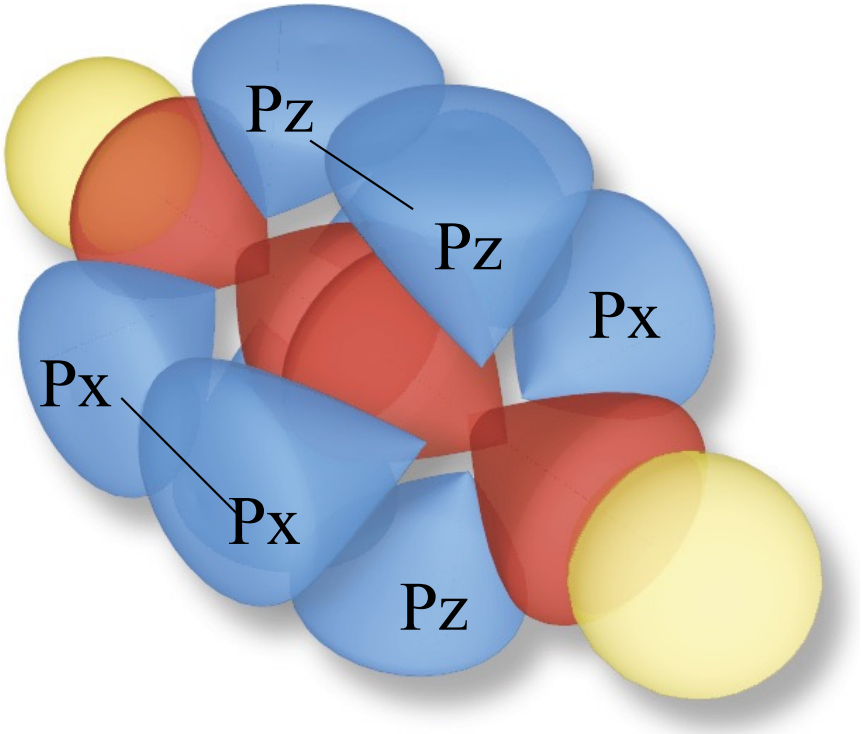


Example: ethyne
(acetylene)

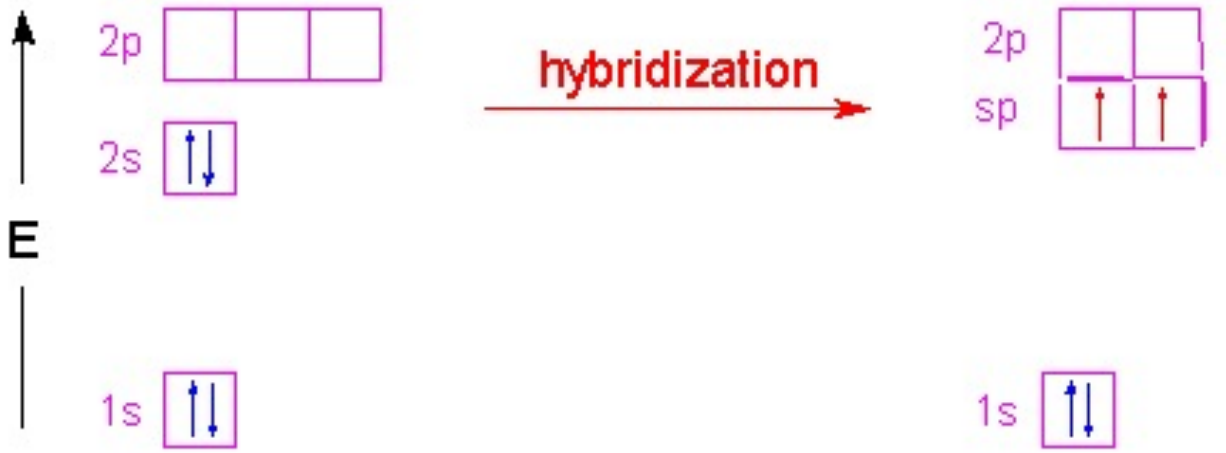
Sp: linear geometry
(180°)

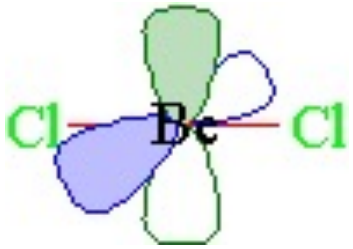


Ethyne

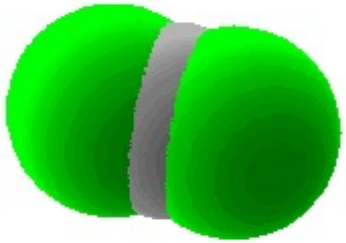
The triple bond can not rotate

$BeCl_2$ exception to the octet rule:



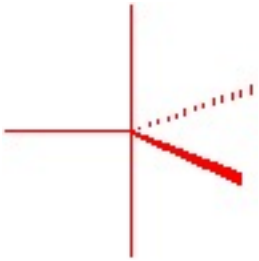


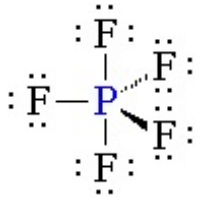
2 Empty p orbital + 2 sp orbitals..



More exceptions to the octet rule: sp^3d e sp^3d^2

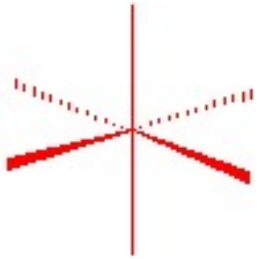
sp^3d

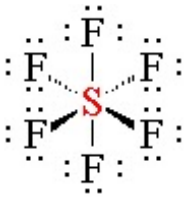




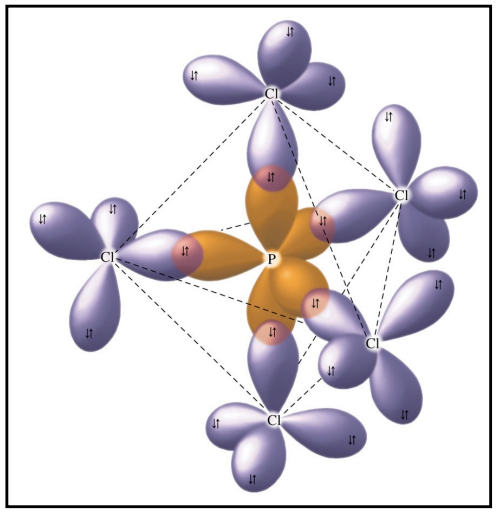
3 angles 120° + 2 orthogonal

sp^3d^2

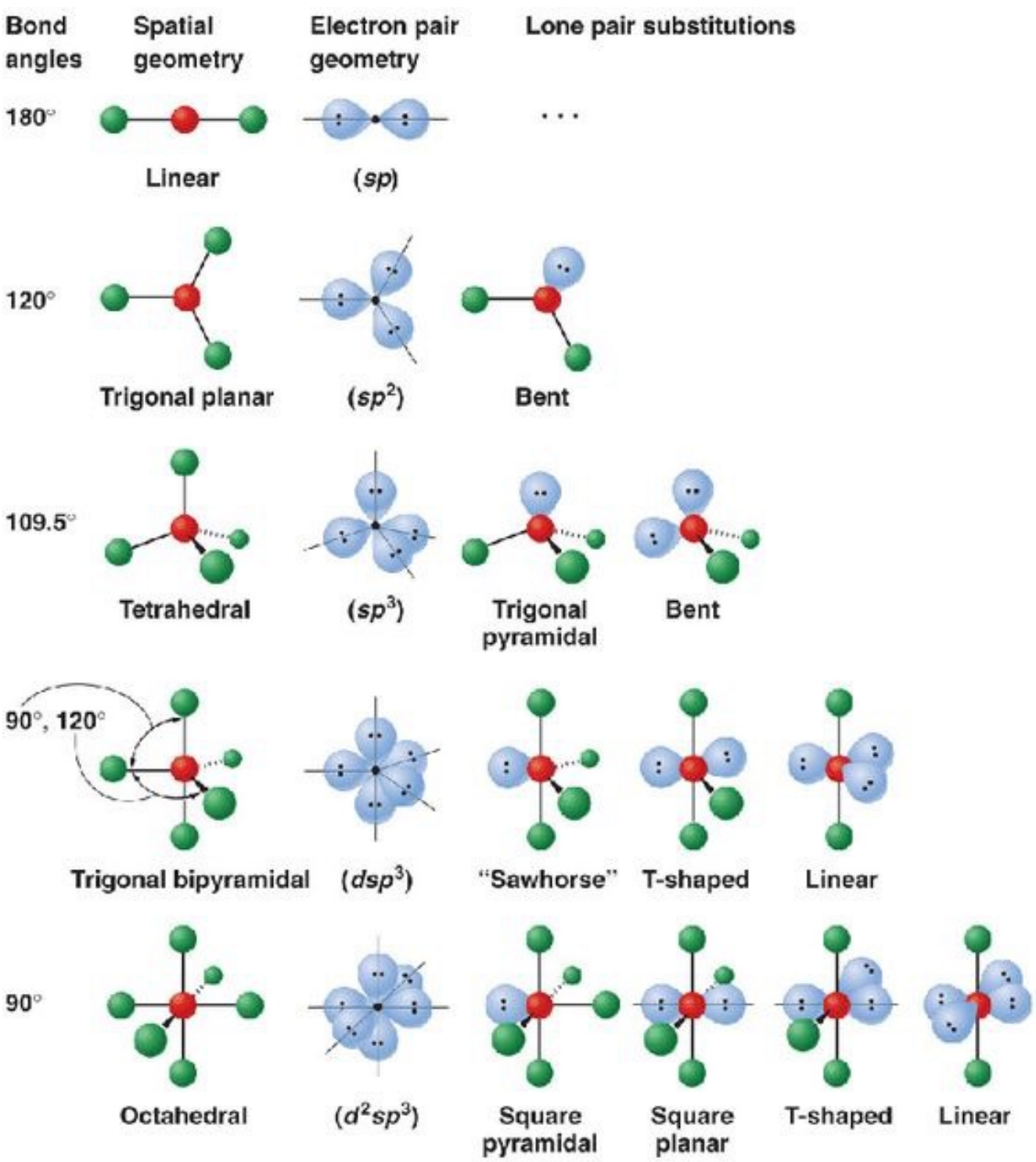


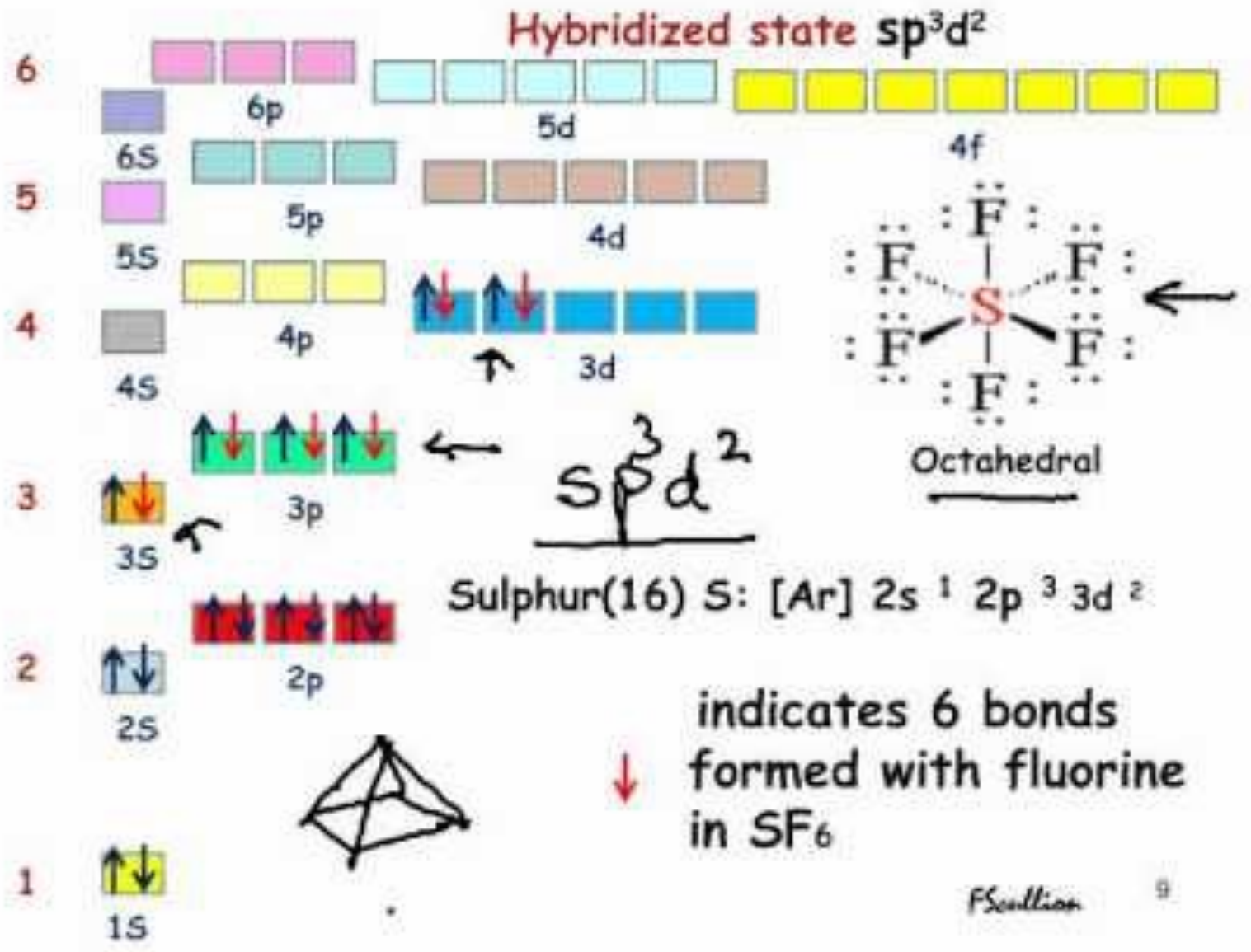


4 angles 90° + 2 orthogonal

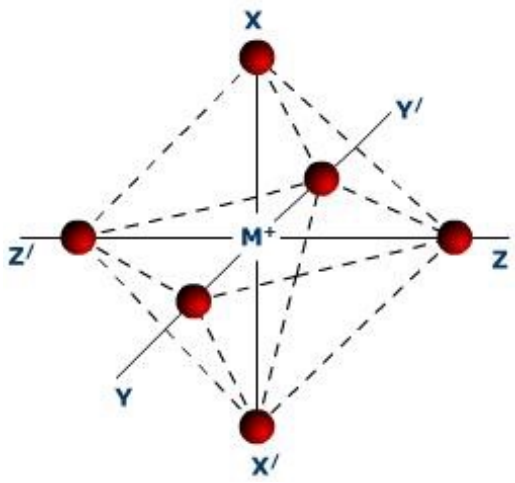


PCl_5

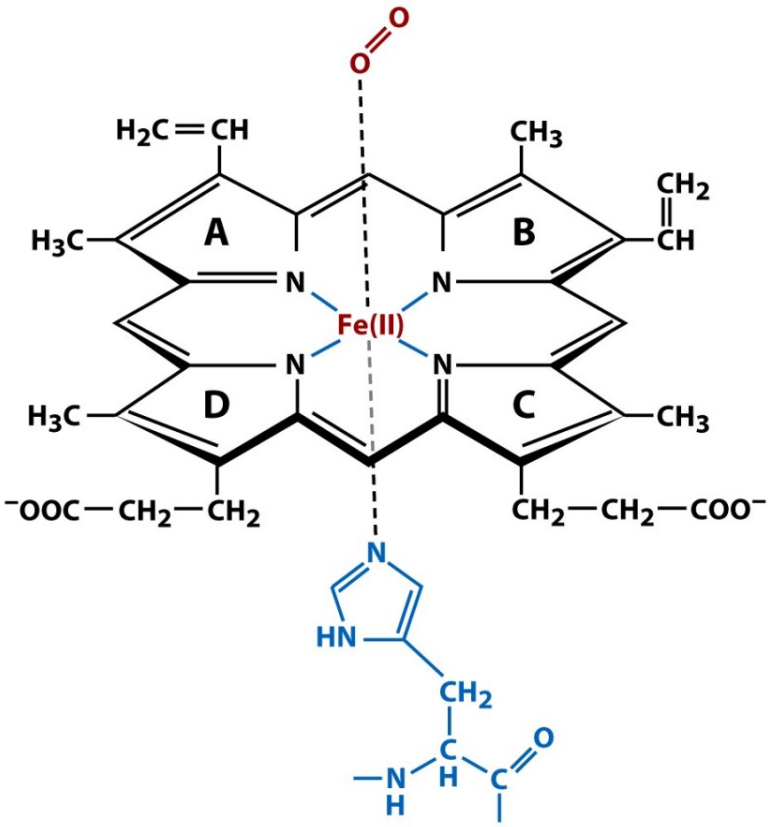



Hybridized state sp³d²
6
6p
5d
4f
6S
5
5p
4d
5S
4
4p
3d
4S
3
3p
3S
2
2p
2S
1
1S
Octahedral
Sulphur(16) S: [Ar] 2s ¹ 2p ³ 3d ²
indicates 6 bonds formed with fluorine in SF6
FSullivan
9

Octahedral coodination in metals



The heme group in myoglobin and hemoglobin.



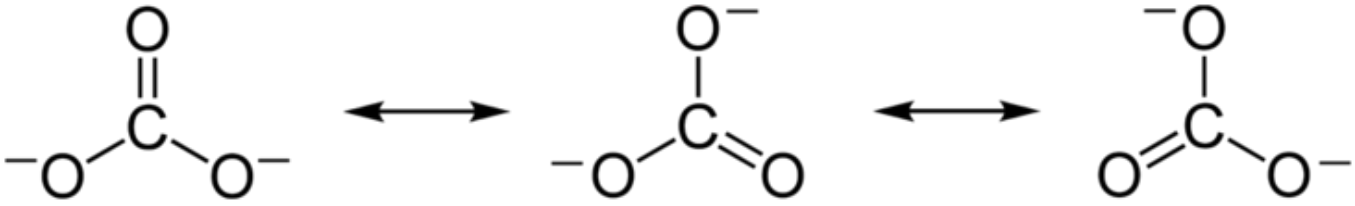
Transition metals have empty orbitals employed in coordination bonds.

Resonance hybrids

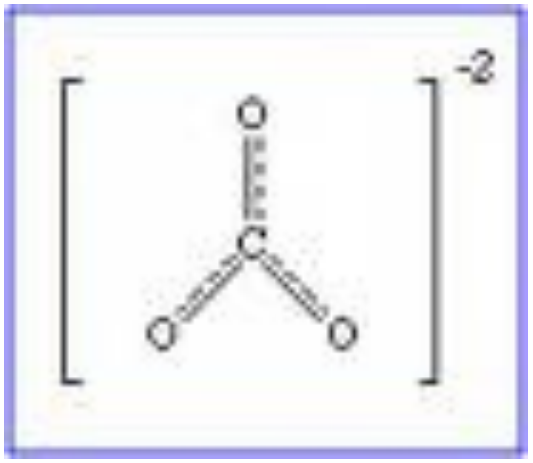
The carbonate ion: $H_2CO_3 + 2H_2O \rightleftharpoons CO_3^{=} + 2H_3O^{+}$

Should have two single bonds and a double one but:
- all bonds have the same length
- The ion shows a stability higher than expected.

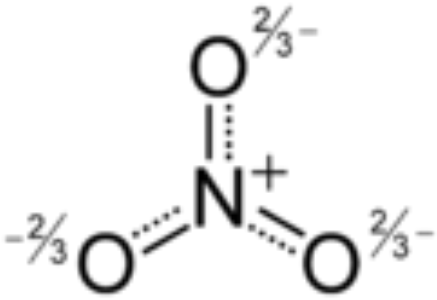
Due to the presence of resonance structures.



The electrons of the double bond (π) are delocalized in the molecule.

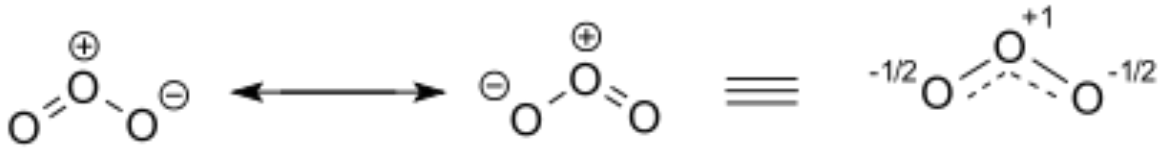


Electron delocalization lowers the potential energy of the substance and thus makes it more stable than any of the contributing structures. The difference between the potential energy of the actual structure and that of the contributing structure with the lowest potential energy is called the resonance energy or delocalization energy.

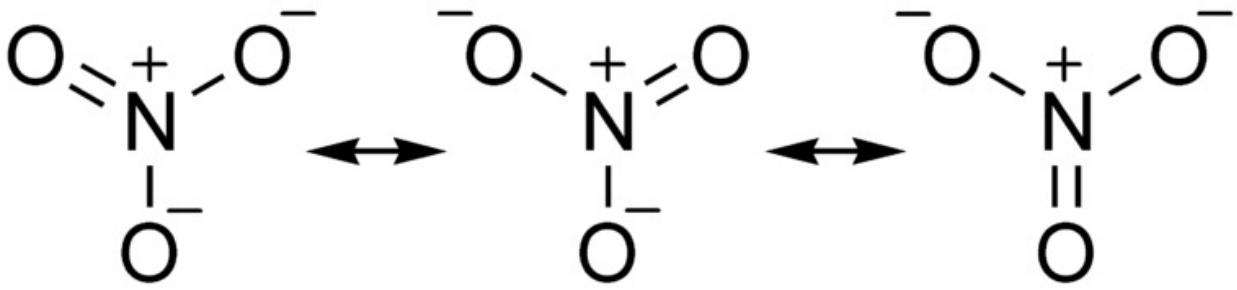


Nitrate ion

The greater the number of contributing structures, the more stable the molecule. This is because the more states at lower energy are available to the electrons in a particular molecule, the more stable the electrons are. Also the more volume electrons can occupy at lower energy the more stable the molecule is.

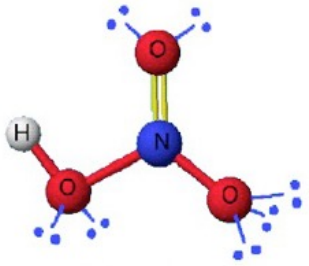


Ozone (O_3)



Nitrate, from the dissociation of nitric acid.

…and countless carbon compounds.



Nitric Acid, HNO_3