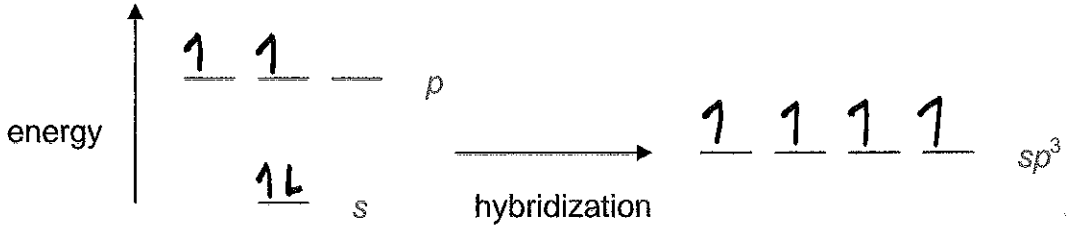
Key

Worksheet 14 - Hybridization

When atoms bond to form molecules, they use **molecular orbitals**. These are formed through the **hybridization** of the **atomic orbitals** that we have already discussed, ***s***, ***p***, and ***d*** orbitals.

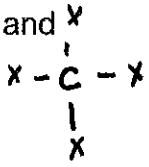
The **hybridized molecular orbitals** have different shapes and energy levels than the **atomic orbitals**. The number of molecular orbitals created by hybridization depends on the number of atomic orbitals that are mixed to form them.

In forming sp^3 hybridized orbitals, **four** atomic orbitals are mixed, one *s* and three *p*. The energy diagram for this process is shown below. The hybridized orbitals are higher in energy than the *s* orbital, but lower in energy than the *p* orbitals.



atomic orbitals **hybridized orbitals**

Carbon has 4 valence electrons. Add these electrons to the atomic and molecular orbitals. This hybridization gives **tetrahedral geometry**.



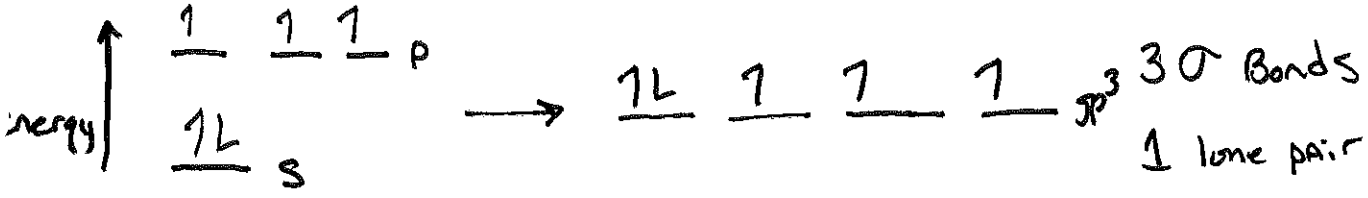
With this hybridization, C will form **four equivalent σ bonds**.

Draw a similar energy diagram for sp^3 hybridized **oxygen**.

How many σ bonds will be formed? 2 σ

How are the other sp^3 orbitals used? lone pair of e⁻

Do the same for sp^3 hybridized **nitrogen**.

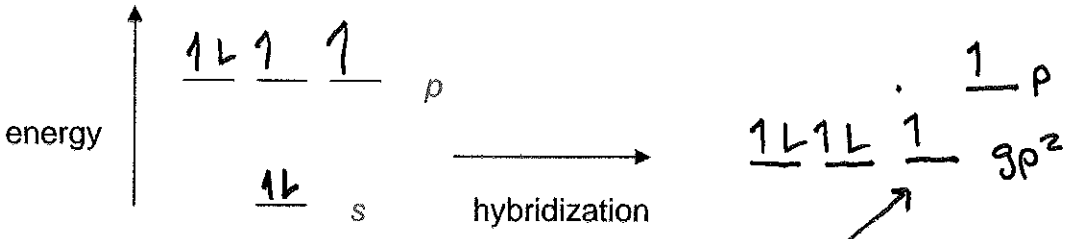


Key

In some Lewis structures, there are only **three** equivalent bonds formed. To create three equivalent hybridized orbitals, mix **three** atomic orbitals.

Draw and name the orbitals formed in this hybridization, then add the electrons for **sulfur**. Since the hybridized orbitals are close in energy, every orbital is filled with one electron before electrons are paired. !

Sulfur



The hybridized orbitals will form 1 σ bond(s).

The unhybridized orbital will form 1 π bond(s).

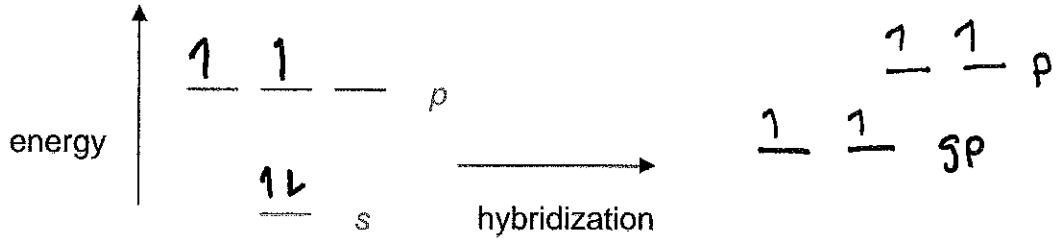
There will be 2 lone pair(s). (same in Both)

This hybridization gives **trigonal planar** geometry.

In **linear** molecules, like CO_2, the central atom has only **two** equivalent bonding orbitals. Draw the energy levels and name the orbitals formed in this hybridization.

:O::C::O:

Linear

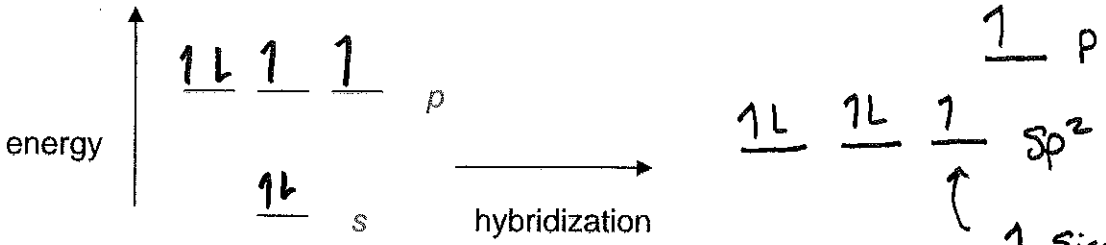


everyone gets 1e since close in energy level

Fill in the electrons for carbon and determine the number and typed of bonds formed. :O::C::O: 2 sigma + 2 π Bonds

In CO_2, determine the hybridization of the **oxygen** atoms. Complete the energy diagram for the oxygens. Draw the structure of CO_2.

:O=C=O:



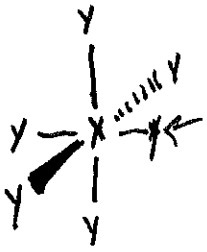
1 Sigma Bond
1 π Bond

Key

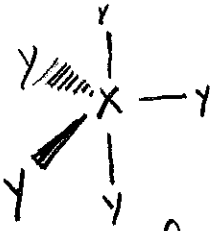
– energy Level

In atoms with n=3 or larger, the *d* orbitals can also be hybridized. In molecules with **five** molecular orbitals, **five** atomic orbitals are mixed:

d + S + P + P + P



This will give **trigonal bipyramidal** geometry and is called ***dsp*^{3}** hybridization.



Finally, molecules with **octahedral** geometry, will have 6 molecular orbitals. This hybridization is called d^2sp^3.

d + d + s + p + p + p

Shown below is a portion of the chart from **Worksheet 13**. Fill in the **hybridization** for each of the compounds.

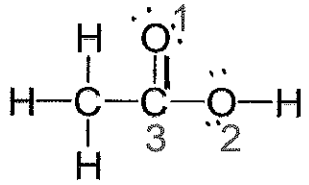
compound	bonds	lone pairs	geometry	shape	hybridization
SF_6	6	0	octahedral	octahedral	d^2sp^3
NH_3	3	1	tetrahedral	trigonal pyramidal	sp^3
ICl_4^-	4	2	octahedral	square planar	d^2sp^3
CF_4	4	0	tetrahedral	tetrahedral	sp^3
SO_3	3	0	trigonal planar	trigonal planar	sp^2
SF_4	4	1	trigonal bipyramidal	seesaw	dsp^3
CO_2	2	0	linear	linear	sp
H_2O	2	2	tetrahedral	V-shaped	sp^3
NO_2^-	2	1	trigonal planar	V-shaped	sp^2

Key

Fill in the chart below and then complete the Lewis structures for the molecules shown below and fill in those charts.

element	Lewis symbol	# bonds	# lone pairs
C		4	0
N		3	1
H		1	0
O		2	2
Halogen		1	3

#1



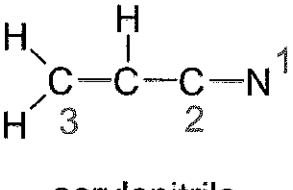
acetic acid

σ bonds 7

π bonds 1

atom #	bond angle	hybridization
1 :O=	120°	sp^2
2 -O-	109°	sp^3
3 -C=	120°	sp^2

#2



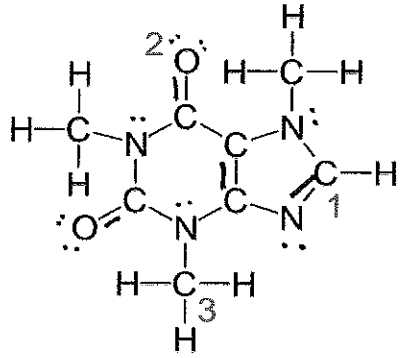
acrylonitrile

σ bonds 6

π bonds 3

atom #	bond angle	hybridization
1 ≡N:	180°	sp
2 -C≡	180°	sp
3 =C=	120°	sp^2

#3



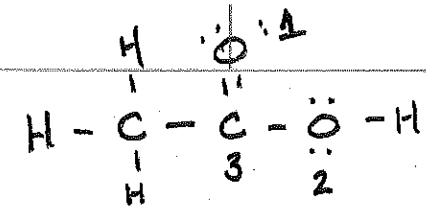
caffeine

σ bonds 25

π bonds 4

atom #	bond angle	hybridization
1 -C=	120°	sp^2
2 :O=	120°	sp^2
3 -C-	109	sp^3

Key



← 1π

1 Atom

#1 O (double bond, 2 lone pairs)

↑ 1⇂ 1 1 p
1⇂ s

→ 1⇂ 1⇂ 1 sp^2, 1 p

1σ

sp^2

1 sigma
1π

O=C (−C−) Trigonal Planer

Steric # = 3
No lone pair
120°

Atom

#2 −O− (2 lone pairs)

2 sigma
2 lone pair

↑ 1⇂ 1 1 p
1⇂ s

→ 1⇂ 1⇂ 1 1 Sp^3

2 sigma
2 lone pair

−X− (2 lone pairs) steric # = 4
2 lone pair = Bent
109°

Atom

#3 −C− (double bond)

3 sigma
1π

↑ 1 1 _ p
1⇂ s

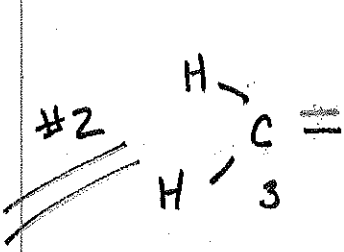
→ 1 1 1 sp^2, 1

1π
3 sigma

−X− (double bond) Steric # = 3
No lone pair
∴ Trigonal planer = 120°

Key

#2

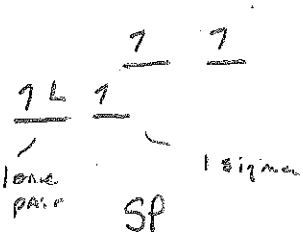


6 Sigma
3 pi

Atom 1

$\equiv N:$

1 sigma
2 pi
1 lone pair



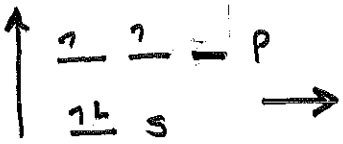
2 Pi

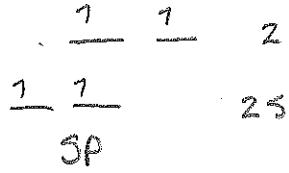
X Linear
180°

Atom 2

$-C\equiv$

2 sigma
2 pi

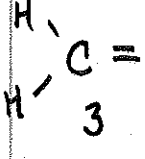




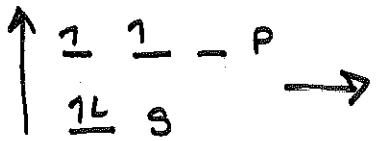
2 pi
2 Sigma

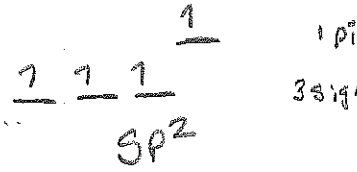
— X — Linear

Atom 3



3 Sigma
1 pi





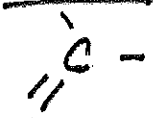
1 pi
3 Sigma

steric # 3
No lone pair ⇒ Trigonal Planer
≈ 120°

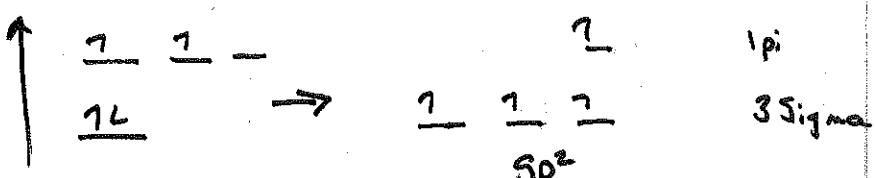
Key

#3 Caffeine

Atom 1



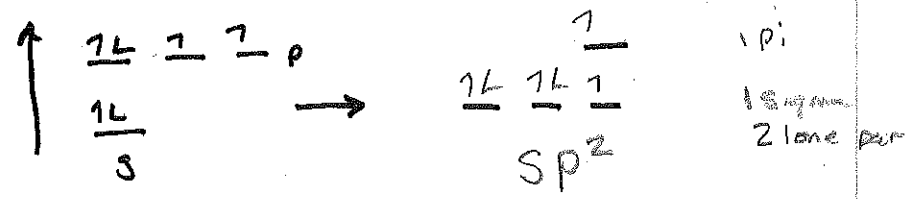
3 sigma
1 pi



Steric # 3 ⇒ Trigonal Planer ∴ 120°
No lone pairs

Atom 2

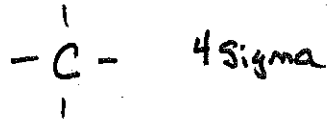
1 Sigma
1 pi
2 lone pair



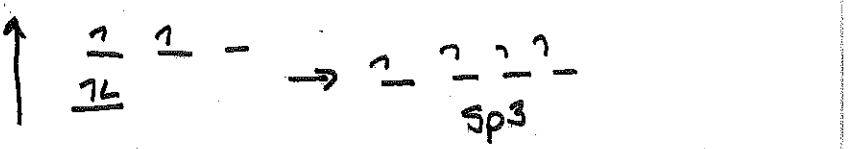
steric # = 3
2 lone pair

But Sp^2 is Trigonal planer ∴ 120°

Atom 3

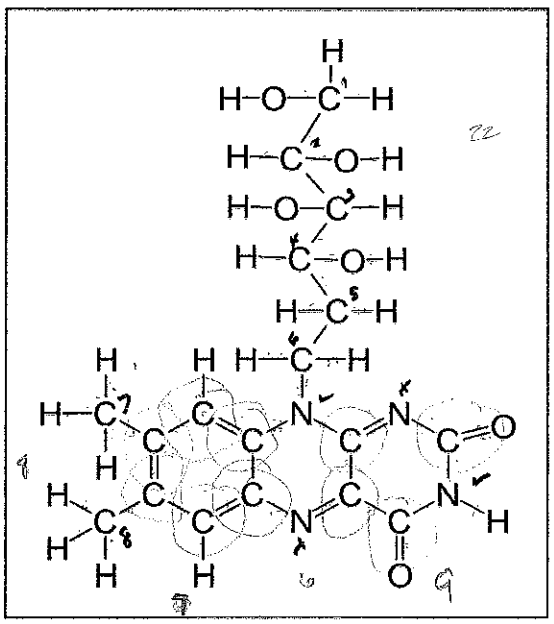


4 Sigma



steric # 4 Tetrahedral
∴ 109°

Key



The molecule shown to the left is riboflavin (vitamin B2). Answer the following questions about its structure.

a) how many carbons are sp^3 hybridized? 8

sp^2 hybridized? 10

sp hybridized? 0

b) How many nitrogens are sp^3 hybridized? 2 ✓

sp^2 hybridized? 2 ×

sp hybridized? 0

c) How many oxygens are sp^3 hybridized? 4

sp^2 hybridized? 2

sp hybridized? 0

d) How many σ bonds are there in total? 52

e) How many π bonds are there in total? 7

The acetate ion, $C_2H_3O_2^-$, has both oxygens bonded to the same carbon.

a) Draw the Lewis structure and all resonance forms.

b) Label the hybridization around each carbon.

c) Pick one resonance structure and label the hybridization of each oxygen.

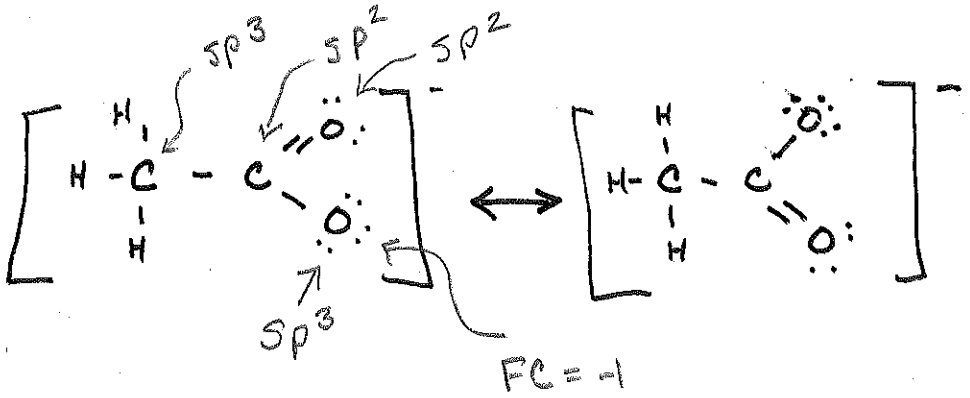
d) How many σ and π bonds are present?

e) Which atom carries the formal negative charge?

Key

$C_2H_3O_2^-$

C 2×4 = 8
H 3×1 = 3
O 2×6 = 12
-e = 1
24 Ve



d) 6 Sigma Bonds

1 pi Bond

e) which Atom has Negative Charge?

	C	C	=O:	−O:
Formal charge	4	4	6	6
	-4	-4	-6	-7
	0	0	0	-1