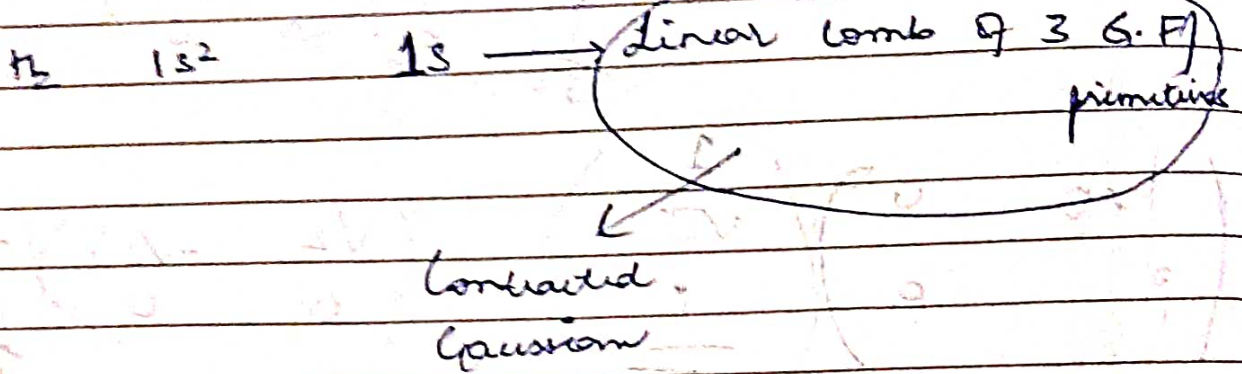


# # Basis Set

1) Minimal Basis Set : STO - nG eg STO - 3G



3 primitives & 1 contracted function

C  $1s^2$   $2s^2$   $2p^2$  STO - 3G

1s 2 9P

2s 3 9P

2p<sub>x</sub> 3 9P

2p<sub>y</sub> 3 9P

2p<sub>z</sub> 3 9P

(Pople type Basis Set)

C  $1s^2$   $2s^2$   $2p^2$

(3)  
(3C)

(3)  
(1P)

(3C)  
(3C)

L.C. of 3 Gaussian orbitals

# primitives = 3

$$c_1 G_1 + c_2 G_2 + c_3 G_3$$

15P  
5 C.F.

for carbon

2p<sub>x</sub> (3)

2p<sub>y</sub> (3)

2p<sub>z</sub> (3)

# primitives = 9

3 contracted fns



	6s	1s <sup>2</sup>	2s <sup>2</sup>	2p <sup>6</sup>	3s <sup>2</sup>	3p <sup>6</sup>	4s <sup>2</sup>	3d <sup>7</sup>
q.p		3	3	9	3	9	3	15
c.p		1	1	3	1	3	1	5

2) Split-Valence Basis Set  $\begin{cases} \text{double-zeta} \\ \text{triple-zeta} \end{cases}$

$3-21(G)$   $\begin{cases} \text{Gaussian} \\ \text{Double Zeta} \end{cases}$  polarized  
diffused

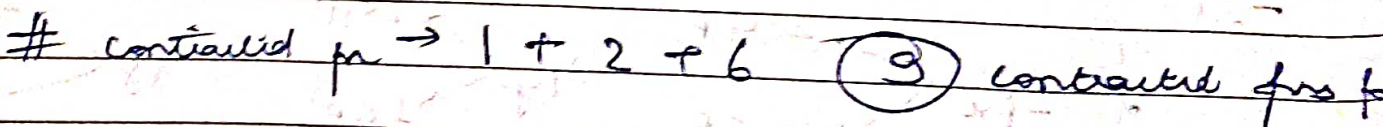
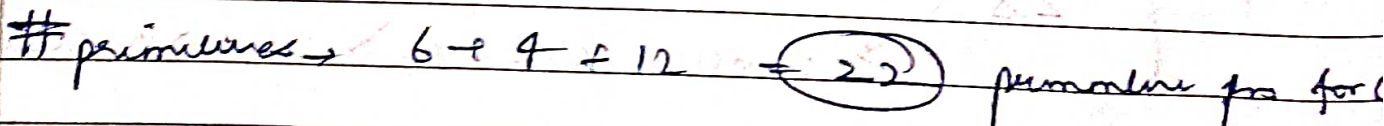
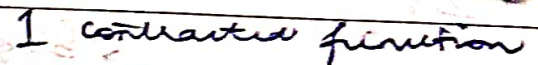
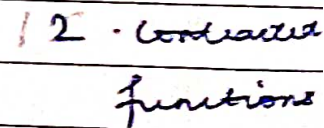
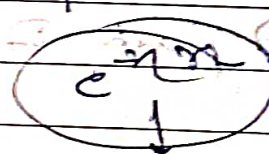
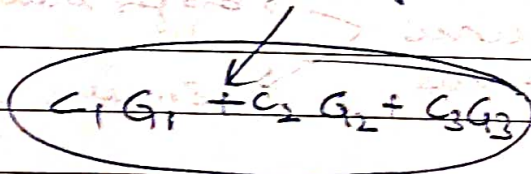
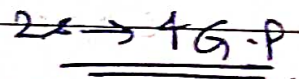
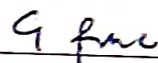
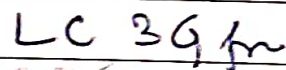
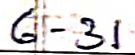
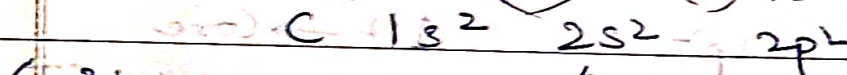
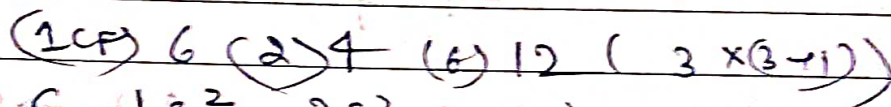
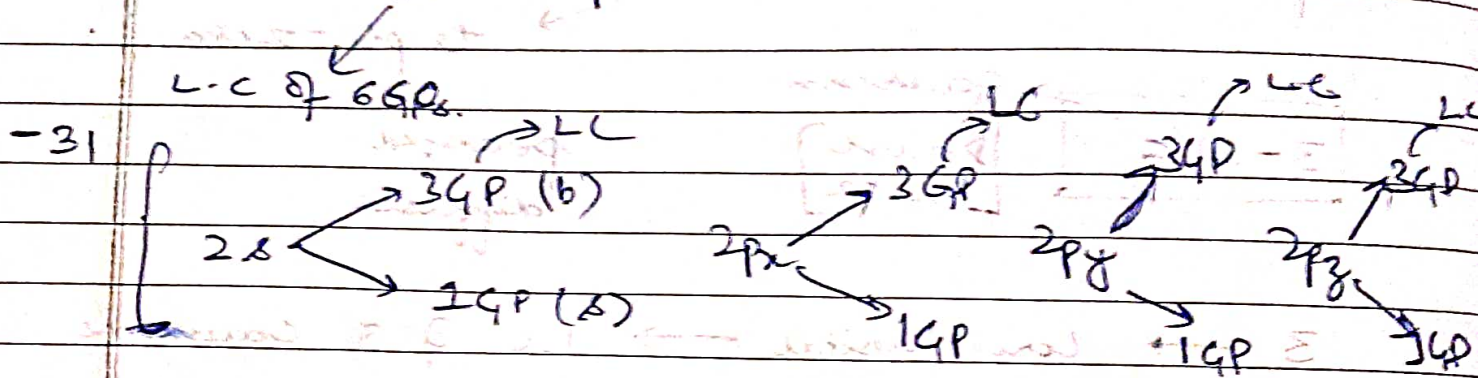
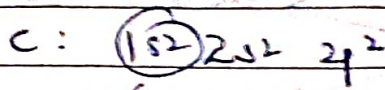
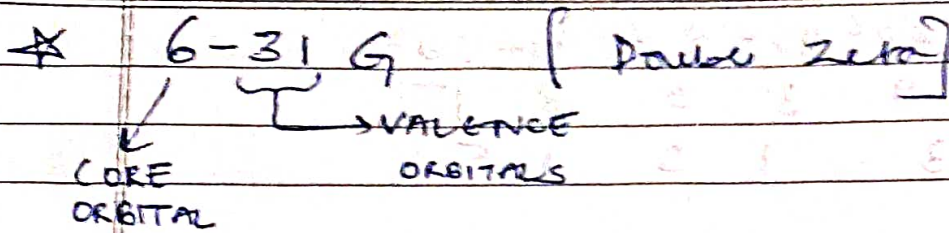
3  $\rightarrow$  Core orbital  $\rightarrow$  LC of 3 Gaussians  
 $\Rightarrow$  STO 3G for the core orbital

C  $1s^2 2s^2 2p^2$   $1s^2 \rightarrow$  Core  
 $\rightarrow$  Just like STO 3G  
i.e. LC of 3 Gaussian fns.

21  $\Rightarrow$  each of valence orbitals  $\begin{cases} \text{bigger Slater fn} \\ \text{smaller Slater fn} \end{cases}$

21  $\left\{ \begin{array}{l} 2s \begin{cases} \text{bigger Slater fn} \rightarrow 2 \text{ Gaussians} \\ \text{smaller Slater function} \rightarrow 1 \text{ Gaussian} \end{cases} \end{array} \right.$

21  $\left\{ \begin{array}{l} 2p_x \begin{cases} 2 \text{ GP} \\ 1 \text{ GP} \end{cases} \\ 2p_y \begin{cases} 2 \text{ GP} \\ 1 \text{ GP} \end{cases} \\ 2p_z \begin{cases} 2 \text{ GP} \\ 1 \text{ GP} \end{cases} \end{array} \right.$



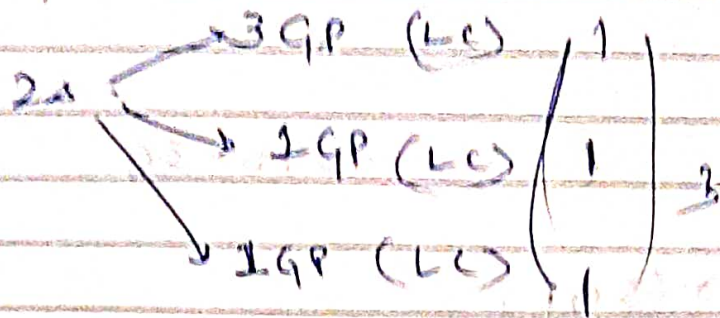


# 6-311G [Triple 2d] C: 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>2</sup>

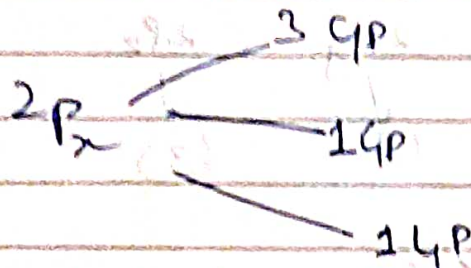
C: (1s<sup>2</sup>) 2s<sup>2</sup> 2p<sup>2</sup>

6GP (1) (2) (3)

$$3 \times 5 = 5 + 6$$



$$15 = 11 + 4$$



# primitives = 26  
# contracted fn = 13

6-31G\* : 6-31(d) 6-31(d,p) → 6-31G\*  
6-311G\* : 6-311(d) 6-311(d,p) → 6-311G\*

Co: 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> 3s<sup>2</sup> 3p<sup>6</sup> 4s<sup>2</sup> 3d<sup>7</sup>  
core valence

6-31G(d) / 6-31G\*

C: 1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>2</sup> l = 1 → include d functions also  
include next higher l value orbital

for Co → include f (l = 3) functions  
(l = 2 highest)



6-31 G(m, p) / 6-31 G \*\*

$H \rightarrow 1s$  ,  $\boxed{l=1}$  (only for H, include p)  
 include  
 Just include next higher l orbitals  
 for 1s, 2s orbitals

\* Molecules

# H2O STO-3G

$H \ 1s \rightarrow (3G, P)$   
 $H \ 1s \rightarrow (3G, P)$   
 $O \ 1s \ 2s \ 2p_x \ 2p_y \ 2p_z$   
 $\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow$   
 $(3) \quad (3) \quad (3) \quad (3) \quad (3)$

memo

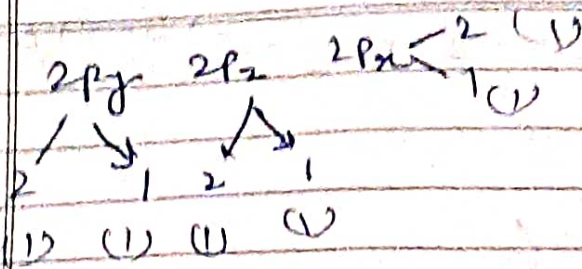
3 Gaussians  $\rightarrow$  16 TO contracted Gauss. type of orbitals.

# G. P    # C. F. L =

21    7

memo

#	<chem>CH2O</chem> / <chem>HCHO</chem>	STO-3G	3-21 G
		STO-3G	3-21 G
	$H \ (1s) : (3) : (1)$	$H \ (1s) \rightarrow 2GP \ (1) \ 3GP \ 2F$	
	$H \ (1s) : (3) : (1)$	$H \ (1s) \rightarrow 2GP \ (1) \ 3GP \ 2GP$	
	$C \ (1s) : (3) : (1)$	$C \ (1s) \rightarrow 3 \ 1$	
	$(2s) : (3) : (1)$	$2s \rightarrow 2GP \ 3 \ 2$	
	$2p : (9) : (3)$	$2p \rightarrow 2GP \ 3 \ 2$	
	$O \ (1s) : (3) : (1)$	$O \ (1s) \rightarrow 3 \ 2$	
	$(2s) : 3 : (1)$	$2s \rightarrow 2GP \ 3 \ 2$	
	$2p : (9) : (3)$	$2p \rightarrow 2GP \ 3 \ 2$	
	<u>36</u> <u>12</u>		



9

6



3

2

0

1s

3

1

2s

3

2

2p

9

6

1.2.3

36

36

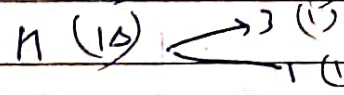
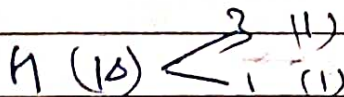
22

#

CH2O

6-31G

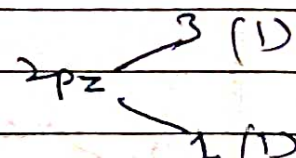
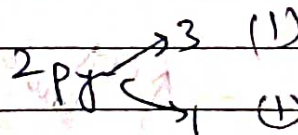
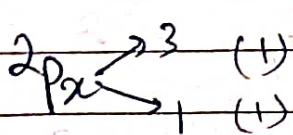
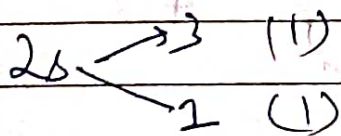
+ 2



C (1s)

6s

(1)



4 2 (CGTO)

4 2

4 2

0 1s

1s → 6

(1)

2s → 2

(1)

2p → 3

(1)

2p → 1

(1)

same

for 2py 2pz

(2px → 3)

(1)

(2px → 1)

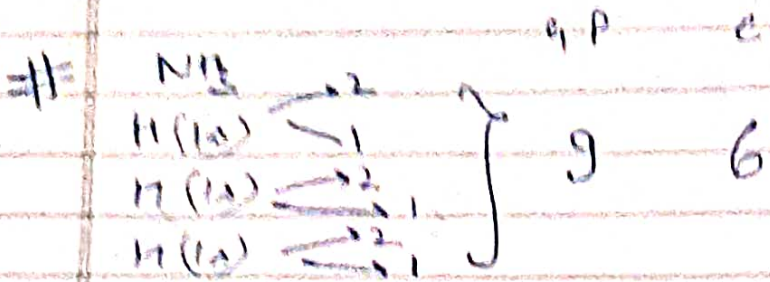
(1)

# primitives = 52

# contracted functions = 22



6-311 9 for  $\text{CH}_2\text{O}$  &  $\text{NH}_3$  → 3-219



N	1s	3	1
	2s	3	2
	2p <sub>x</sub>	3	2
	2p <sub>y</sub>	3	2
	2p <sub>z</sub>	3	2

24    15

# 3-21  $\text{G}(\text{d}, \text{p})$      $\text{CH}_4$     3-219\*\*

H	$\begin{matrix} \swarrow 2 \\ \searrow 1 \end{matrix}$	Gp	CF	4H	Gp	CF
		3	2		4x3	4x2
+1p function				1s	(without p)	

Gp	C	H p	4(3)	4(3)
3	3			

2s	→ 2	15	C	3	1
	→ 1		1s	3	2

2p	→ 2	17	2p	3x3	3x2
	→ 1				without d

4	5	3	5
---	---	---	---

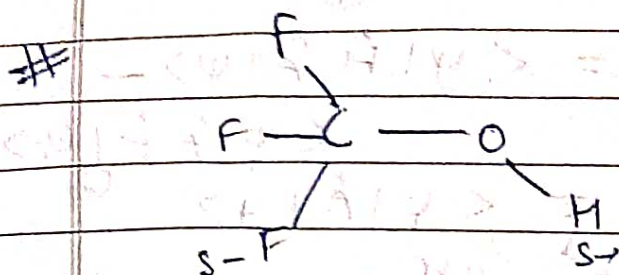
21  
12/3  
3/2

papergrid

Date: / /

# HCHO 3-21 G\*\*

6-311 G(d,p) | 6-311 G\*\*



Bond stretching = 5 bonds

bending = 7 terms

3 F-C-O bonds

1 C-O-H bond

3 F-C-F bond

Torsion → 3 F-C-OH

7 angles.

3 Vonder Waals

3 electrostatic terms