Overview of commonly used basis sets

STO - 3G Basis

Contracted Basis

Each s and p basis function is represented by 3 gaussian primitives

(6s3p) → [2s1p]

1s basis function		*2s basis function*		*2p basis function*	
α_1	d_1	α_4	ds_4	α_4	dp_4
α_2	d_2	α_5	ds_5	α_5	dp_5
α_3	d_3	α_6	ds_6	α_6	dp_6

$$s = \sum_{\mu=1}^{3} g_\mu d_{\mu 1s} \qquad 2s = \sum_{\mu=4}^{6} g_\mu d_{\mu 2s}$$

$$2p_\alpha = r_\alpha \sum_{\mu=4}^{6} g_\mu d_{\mu 2p}$$

NOTE: The 2s and 2p basis functions share the same exponents. They are said to be in the same shell.

Formaldehyde in an STO-3G basis

atom	primitives	contracted
H1	3s	1s
H2	3s	1s
C	6s, 3p	2s, 1p
O	6s, 3p	2s, 1p
total functions	36	12

in the primitive - uncontracted basis

$$\varphi_i = \sum_{\mu=1}^{36} g_\mu c_{\mu i} \quad ; \; i=1,36$$

while in the contracted (STO-3G) one has

$$\varphi_i = \sum_{\mu=1}^{12} \chi_\mu c_{\mu i} \; ; \; i=1,12$$

3-21 Basis for a First Row Atom

There are three s basis functions

The 1s basis function is a sum of three s gaussian functions with exponents
$\alpha_1, \alpha_2, \alpha_3$

$$s = \sum_{\mu=1}^{3} g_\mu d_{\mu 1s}$$

The 2s basis function is a sum of two s gaussian functions with exponents α_4, α_5

$$2s = \sum_{\mu=4}^{5} g_\mu d_{\mu 2s}$$

The 3s basis function is a single gaussian with exponent α_6

$$3s = g_6$$

There are two p basis functions

The first is a sum of two p gaussians with exponents α_4 and α_5

$$p = \sum_{\mu=4}^{5} g_\mu d_{\mu 1p}$$

The second p basis function is a single p gaussian with exponent α_6

$$2p = g_6$$

Formaldehyde in a 3-21 Basis

atom	primitives	contracted
H1	3s	1s
H2	3s	1s
C	6s,3p	3s,2p
O	6s,3p	3s,2p
total	36	20

Formaldehyde in a 6-21 Basis

atom	primitives	contracted
H1	3s	1s
H2	3s	1s
C	9s,3p	3s,2p
O	9s,3p	3s,2p
total	42	20

Polarization Functions

H atom	add functions of p symmetry
B - Ne	add functions of d symmetry
	designate polarization functions with a *
3-21G*	a 3-21 G basis with 6 d's on elements B - Ne
3-21G**	3-21 G basis with a p set on each Hydrogen atom

Formaldehyde in a 3-21 G** basis

atom	primitives	contracted
H1	3s,1p	2s,1p
H2	3s,1p	2s,1p
C	6s,3p,1d	3s,2p,1d
O	6s,3p,1d	3s,2p,1d
total	54	40