Carbon Basis Sets

The 1s and 2s orbitals are expressed as linear combinations of s gaussians

$$\phi_{1s} = \sum_{\mu=1}^{n_s} \chi_\mu C_{\mu,1s} \text{ and } \phi_{2s} = \sum_{\mu=1}^{n_s} \chi_\mu C_{\mu,2s}$$

where n_s is the number of gaussians in the expansion,

$\chi_\mu = \left(2/\pi\right)^{3/4} \alpha_\mu^{3/4} e^{-\alpha_\mu r^2}$ is the s gaussian function

and $C_{\mu,1s}$ *and* $C_{\mu,2s}$ are the expansion coefficients determined by the Hartree-Fock equations. Note that the 1s and 2s orbitals are being expanded with the same set of gaussians. The only difference between the 1s and 2s orbitals will be the expansion coefficients

The 2p orbitals are also expressed as linear combinations of gaussians with the $2p_x$ orbital given by

$$2p_x = x \sum_{\mu=1}^{n_p} \chi_\mu C_{\mu,2p}$$

where n_p is the number of gaussians in the expansion, and

$\chi_\mu = 2\left(2/\pi\right)^{3/4} \alpha_\mu^{5/4} e^{-\alpha_\mu r^2}$ is the p gaussian function . Note that all 3 of the p orbitals will have the same radial function and differ only in their orientation, x, y, z.

The following table lists the exponents and coefficients for two sets of approximate Hartree-Fock orbitals, a (6s, 3p) and a (9s, 5p) expansion.

(6s, 3p) expansion Energy = --37.618754 au

orbital symmetry		1s	2s
orbital energy(au)		-0.11319867D 02	-0.67763325D 00
μ	exponent	$C_{\mu,1s}$	$C_{\mu,2s}$
1	0.10870968D 04	0.65890782D-02	0.13305455D-02
2	0.16386717D 03	0.48334667D-01	0.10804301D-01
3	0.37409003D 02	0.20701690D 00	0.42542866D-01
4	0.10518070D 02	0.47841396D 00	0.15006002D-00
5	0.33207801D 01	0.40229784D 00	0.12488790D 00
6	0.29343569D-00	0.13204377D-01	-0.10412835D01

orbital symmetry		2p
orbital energy(au)		-0.41193189D 00
μ	exponent	$C_{\mu,2p}$
1	0.42016899D 01	0.11192092D 00
2	0.85849135D 00	0.46241685D 00
3	0.20206301D 00	0.62534638D 00

(9s, 5p) expansion Energy = --37.685269 au

orbital symmetry		1s	2s
orbital energy(au)		-0.24775901D 01	-0.19630374D 00
μ	exponent	$C_{\mu,1s}$	$C_{\mu,2s}$
1	0.42403098D 04	0.12152226D-02	0.25753074D-03
2	0.63777827D 03	0.92731586D-02	0.20056132D-02
3	0.14674534D 03	0.45279235D-01	0.97036547D-02
4	0.42531428D 02	0.15492334D 00	0.36142023D-01
5	0.14184804D 02	0.35808349D 00	0.89166352D-01
6	0.51756943D 01	0.43427160D 00	0.17542094D 00
7	0.20072531D 01	0.14932812D 00	0.54345495D-01
8	0.49677422D 00	0.30145799D-02	-0.57313491D 00
9	0.15348718D 00	0.12585789D-03	-0.54851147D 00

orbital symmetry		2p
orbital energy(au)		-0.43249574D 00
μ	exponent	$C_{\mu,2p}$
1	0.18099144D 02	0.14760512D-01
2	0.39769145D 01	0.91649350D-01
3	0.11450768D 01	0.30392714D 00
4	0.36188831D 00	0.50711806D 00
5	0.11460548D 00	0.31988309D 00