Lithium Basis Sets

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

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

where n_g 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

6s expansion Energy = -7.4278571 au

orbital symmetry		1s	2s
orbital energy(au)		-0.24762539D 01	-0.19500016D 00
μ	exponent	$C_{\mu,1s}$	$C_{\mu,2s}$
1	0.26627469D 03	0.63815921D-02	0.97512293D-03
2	0.40048144D 02	0.47000421D-01	0.73539994D-02
3	0.90287102D 01	0.20002380D 00	0.31990919D-01
4	0.24329989D 00	0.47913213D 00	0.90309661D-01
5	0.71062733D 00	0.42024154D 00	0.14676226D 00
6	0.47789070D-01	0.10234330D-01	-0.10363603D01

9s expansion Energy = -7.4322865 au

orbital symmetry		1s	2s
orbital energy(au)		-0.24775901D 01	-0.19630374D 00
μ	exponent	$C_{\mu,1s}$	$C_{\mu,2s}$
1	0.92930934D 03	0.13539830D-02	0.21101810D-03
2	0.13999549D 03	0.10276722D-01	0.16186196D-02
3	0.32317344D 02	0.49240471D-01	0.77676845D-02
4	0.94102350D 01	0.16071350D 00	0.26753991D-01
5	0.31647162D 01	0.34368350D 00	0.60653228D-01
6	0.11678191D 01	0.42041736D 00	0.10728203D 00
7	0.45450346D 00	0.17436782D 00	0.10900489D 00
8	0.76477490D-01	0.34563867D-02	-0.55679103D 00
9	0.28694850D-01	-0.50728983D-03	-0.54421138D 00