Helium Basis Sets

The 1s orbital is expressed as linear combinations of s Gaussian functions

$$\phi_{1s} = \sum_{\mu=1}^{M} \chi_\mu C_{\mu,1s}$$

where M 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

$C_{\mu,1s}$ are the expansion coefficients determined by the Hartree-Fock equations..

6s expansion Energy = -2.861153 au

	orbital energy(au)	-0.91763 au
μ	exponent	$C_{\mu,1s}$
1	233.092501	0.002600
2	35.022805	0.019628
3	7.955702	0.091421
4	2.202780	0.272853
5	0.664349	0.478261
6	0.208245	0.306262

7s expansion Energy = -2.861514 au

orbital symmetry		1s
orbital energy(au)		-0.91785 au
μ	exponent	$C_{\mu,1s}$
1	528.390342	0.000940
2	79.275179	0.007219
3	18.036064	0.036011
4	5.080905	0.127882
5	1.607997	0.308474
6	0.536241	0.452874
7	0.183315	0.238915

Convergence as a function of the expansion length

M	1s energy (au)	Total energy (au)
1		-2.300987
2	-0.85890	-2.747066
3	-0.90357	-2.835680
4	-0.91413	-2.855160
5	-0.91687	-2.859895
6	-0.91763	-2.861153
7	-0.91785	-2.861514
8	-0.91792	-2.861625
9	-0.91794	-2.861661
10	-0.91795	-2.861673