

Optional homework #6

Implement an s -type Gaussian-basis-set Hartree–Fock program for polyatomic molecules. Note that $F_0(T)$ is related to the error function, which is an intrinsic mathematical function available in both Fortran and C. Furthermore, since p -type and higher angular momentum Gaussians are derivatives of s -type Gaussians with respect to their origins, they can be approximated by a linear combination of origin-shifted s -type Gaussians.

S. Obara and A. Saika, “Efficient recursive computation of molecular integrals over Cartesian Gaussian functions,” *J. Chem. Phys.*, **84**, 3963 (1986).

J. L. Whitten, “Gaussian lobe function expansions of Hartree–Fock solutions for the first-row atoms and ethylene,” *J. Chem. Phys.*, **44**, 359 (1966).