1 Slater-type orbitals

A real Slater-type orbital (STO) is defined as follows:

$$\chi_{nlm}(\zeta, \mathbf{r}) = N_n(\zeta) R_n(r, \zeta) S_{lm}(\theta, \phi) \tag{1}$$

where

$$N_n(\zeta) = \frac{(2\zeta)^{n+\frac{1}{2}}}{\sqrt{(2n)!}} \tag{2}$$

is the normalization factor,

$$R_n(r, \zeta) = r^{n-1} e^{-\zeta r} \tag{3}$$

is the radial part and $S_{lm}(\theta, \phi)$ is a real spherial harmonic.

2 Overlap integrals

The one-center overlap integrals

$$S_{nlm,n'l'm'}(\zeta, \zeta') = \int \chi^{\star}_{nlm}(\zeta, \mathbf{r}) \chi_{n'm'l'}(\zeta', \mathbf{r}) \mathrm{d}V \tag{4}$$

is the most straightforward molecular integrals and is readily evaluated in spherical coordinates. The integration of the radial part yields

$$\int_0^\infty R_n(\zeta, r) R_{n'}(\zeta', r) r^2 \mathrm{d}r = \frac{(n+n')!}{(\zeta+\zeta')^{n+n'+1}} \tag{5}$$

and using the orthonormality condition of the spherical harmonics, the analytical form of one-center overlap is

$$S_{nlm,n'l'm'}(\zeta, \zeta') = N_n(\zeta) N_{n'}(\zeta') \frac{(n+n')!}{(\zeta+\zeta')^{n+n'+1}} \delta_{ll'} \delta_{mm'} \tag{6}$$