1 BasisSet.py

The function form of the gaussian basis functions is given as:

$$\phi_A(r) = N(x - A_x)^l (y - A_y)^m (z - A_z)^n \exp\left(-\zeta\left(\vec{r} - \vec{A}\right)^2\right)$$

1.1 def N()

Here the normalization, the quantity calculated is:

$$N = \left(\frac{2\alpha}{\pi}\right)^{3/4}\left[\frac{(8\alpha)^{l+m+n}\, l!m!n!}{(2l)!\,(2m)!\,(2n)!}\right]$$

1.2 def bassisset()

This function will build an array with the needed information about the basis set. The array will have the following information:

$$\begin{bmatrix} Idx & x & y & z & \#CONTR & CONTR \end{bmatrix}$$

Idx is the AO index. $\#CONTR$ contains the number of primitive functions in the contracted.
$CONTR$ contains all the information about the primitive functions and have the form:

$$\begin{bmatrix} N & \zeta & c & l & m & n \end{bmatrix}$$

2 MolecularIntegrals.py

The following notation is useful to know for some of the following functions. For the Gaussian product rule:

$$\exp\left(-ax_A^2\right)\exp\left(-bx_B^2\right) = \exp\left(-\mu X_{AB}^2\right)\exp\left(-px_P^2\right)$$

Here:

$$p = a + b$$

$$\mu = \frac{ab}{a+b}$$

$$P_x = \frac{aA_x + bB_x}{p}$$

$$X_{AB} = A_x - B_x$$

$$K_{ab}^{x} = \exp\left(-\mu X_{AB}^2\right)$$

2.1 def Overlap()

Here the overlap integrals between two primitive functions is calculated following the Obara-Saika scheme:

$$S_{i+1,j} = X_{PA} S_{ij} + \frac{1}{2p}\left(i S_{i-1,j} + j S_{i,j-1}\right)$$

$$S_{i,j+1} = X_{PB} S_{ij} + \frac{1}{2p}\left(i S_{i-1,j} + j S_{i,j-1}\right)$$

With the boundary condition that:

$$S_{00} = \sqrt{\frac{\pi}{p}} \exp\left(-\mu X_{AB}^2\right)$$