

**Computational Chemistry Pre-Lab**  
**(Can be done in lab – after my pre-lab talk)**

1. Determine how many basis functions and Gaussian functions are used for a 6-31G calculation on HCl and then for N,N-dimethylacetamide.

2. a). Use Mathcad to explore the Gaussian function,  $e^{-\alpha r^2}$ , by creating a Gaussian function with  $\alpha$  and  $r$  as arguments. Try different values of  $\alpha$ . What effect does  $\alpha$  have?

b). Plot the three Gaussian functions defined by equations 7 and 8 individually on the same plot for a 1s hydrogen electron ( $Z=1$ ). You should create a Mathcad function to generate a Gaussian function with an exponent as a parameter. What effect does the exponent have? The coefficient? Create a Gaussian function that is more spread out, diffuse. Create a variable that is the sum of the three functions above and plot the resulting new function. Overlay the radial part of the Slater function (eq. 5) with  $\zeta=1.24$  and compare these functions. In doing this realize that we are looking at the hydrogen 1s function so  $l=0$  and  $m=0$ . This means that we are thinking of  $Y(0,0,\theta,\phi)$ .

$$Y(0,0,\theta,\phi) = \frac{1}{(4\pi)^{1/2}}$$