

SymPy generated orbital functions

$\phi_0 \rightarrow \phi_{0,0,0}$	
$\phi(\vec{r})$	1
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2ax$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ay$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2az$
$\nabla^2 \phi(\vec{r})$	$2a(2ar^2 - 3)$

Table 1: Orbital expressions gaussians : 0, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_1 \rightarrow \phi_{0,0,1}$	
$\phi(\vec{r})$	z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2az^2 + 1$
$\nabla^2 \phi(\vec{r})$	$2az(2ar^2 - 5)$

Table 2: Orbital expressions gaussians : 0, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_2 \rightarrow \phi_{0,1,0}$	
$\phi(\vec{r})$	y
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ay^2 + 1$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ayz$
$\nabla^2 \phi(\vec{r})$	$2ay(2ar^2 - 5)$

Table 3: Orbital expressions gaussians : 0, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_3 \rightarrow \phi_{1,0,0}$	
$\phi(\vec{r})$	x
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2ax^2 + 1$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axy$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axz$
$\nabla^2 \phi(\vec{r})$	$2ax(2ar^2 - 5)$

Table 4: Orbital expressions gaussians : 1, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_4 \rightarrow \phi_{0,0,2}$	
$\phi(\vec{r})$	z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^2$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$z^2(4a^2r^2 - 14a) + 2$

Table 5: Orbital expressions gaussians : 0, 0, 2. Factor e^{-ar^2} is omitted.