

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.

$\phi_5 \rightarrow \phi_{0,1,1}$	
$\phi(\vec{r})$	yz
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axyz$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2ayz(2ar^2 - 7)$

Table 6: Orbital expressions gaussians : 0, 1, 1. Factor e^{-ar^2} is omitted.

$\phi_6 \rightarrow \phi_{0,2,0}$	
$\phi(\vec{r})$	y^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^2z$
$\nabla^2 \phi(\vec{r})$	$y^2(4a^2r^2 - 14a) + 2$

Table 7: Orbital expressions gaussians : 0, 2, 0. Factor e^{-ar^2} is omitted.

$\phi_7 \rightarrow \phi_{1,0,1}$	
$\phi(\vec{r})$	xz
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2axz(2ar^2 - 7)$

Table 8: Orbital expressions gaussians : 1, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_8 \rightarrow \phi_{1,1,0}$	
$\phi(\vec{r})$	xy
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axyz$
$\nabla^2 \phi(\vec{r})$	$2axy(2ar^2 - 7)$

Table 9: Orbital expressions gaussians : 1, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_9 \rightarrow \phi_{2,0,0}$	
$\phi(\vec{r})$	x^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2y$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^2z$
$\nabla^2 \phi(\vec{r})$	$x^2(4a^2r^2 - 14a) + 2$

Table 10: Orbital expressions gaussians : 2, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_{10} \rightarrow \phi_{0,0,3}$	
$\phi(\vec{r})$	z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^3$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2z(z^2(2a^2r^2 - 9a) + 3)$

Table 11: Orbital expressions gaussians : 0, 0, 3. Factor e^{-ar^2} is omitted.

$\phi_{11} \rightarrow \phi_{0,1,2}$	
$\phi(\vec{r})$	yz^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axyz^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z^2(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2yz(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y(z^2(2a^2r^2 - 9a) + 1)$

Table 12: Orbital expressions gaussians : 0, 1, 2. Factor e^{-ar^2} is omitted.

$\phi_{12} \rightarrow \phi_{0,2,1}$	
$\phi(\vec{r})$	y^2z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2yz(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^2(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2z(y^2(2a^2r^2 - 9a) + 1)$

Table 13: Orbital expressions gaussians : 0, 2, 1. Factor e^{-ar^2} is omitted.

$\phi_{13} \rightarrow \phi_{0,3,0}$	
$\phi(\vec{r})$	y^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^2(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^3z$
$\nabla^2 \phi(\vec{r})$	$2y(y^2(2a^2r^2 - 9a) + 3)$

Table 14: Orbital expressions gaussians : 0, 3, 0. Factor e^{-ar^2} is omitted.

$\phi_{14} \rightarrow \phi_{1,0,2}$	
$\phi(\vec{r})$	xz^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz^2$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xz(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x(z^2(2a^2r^2 - 9a) + 1)$

Table 15: Orbital expressions gaussians : 1, 0, 2. Factor e^{-ar^2} is omitted.

$\phi_{15} \rightarrow \phi_{1,1,1}$	
$\phi(\vec{r})$	xyz
$\vec{i} \cdot \nabla \phi(\vec{r})$	$yz(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xz(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2axyz(2ar^2 - 9)$

Table 16: Orbital expressions gaussians : 1, 1, 1. Factor e^{-ar^2} is omitted.

$\phi_{16} \rightarrow \phi_{1,2,0}$	
$\phi(\vec{r})$	xy^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xy(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axy^2z$
$\nabla^2 \phi(\vec{r})$	$2x(y^2(2a^2r^2 - 9a) + 1)$

Table 17: Orbital expressions gaussians : 1, 2, 0. Factor e^{-ar^2} is omitted.

$\phi_{17} \rightarrow \phi_{2,0,1}$	
$\phi(\vec{r})$	x^2z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xz(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2z(x^2(2a^2r^2 - 9a) + 1)$

Table 18: Orbital expressions gaussians : 2, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_{18} \rightarrow \phi_{2,1,0}$	
$\phi(\vec{r})$	x^2y
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xy(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz$
$\nabla^2 \phi(\vec{r})$	$2y(x^2(2a^2r^2 - 9a) + 1)$

Table 19: Orbital expressions gaussians : 2, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_{19} \rightarrow \phi_{3,0,0}$	
$\phi(\vec{r})$	x^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2(-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^3y$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^3z$
$\nabla^2 \phi(\vec{r})$	$2x(x^2(2a^2r^2 - 9a) + 3)$

Table 20: Orbital expressions gaussians : 3, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_{20} \rightarrow \phi_{0,0,4}$	
$\phi(\vec{r})$	z^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^4$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^4$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2z^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2z^2(z^2(2a^2r^2 - 11a) + 6)$

Table 21: Orbital expressions gaussians : 0, 0, 4. Factor e^{-ar^2} is omitted.

$\phi_{21} \rightarrow \phi_{0,1,3}$	
$\phi(\vec{r})$	yz^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axyz^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z^3(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$yz^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2yz(z^2(2a^2r^2 - 11a) + 3)$

Table 22: Orbital expressions gaussians : 0, 1, 3. Factor e^{-ar^2} is omitted.

$\phi_{22} \rightarrow \phi_{0,2,2}$	
$\phi(\vec{r})$	y^2z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2yz^2(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^2z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$y^2(4a^2r^2z^2 - 22az^2 + 2) + 2z^2$

Table 23: Orbital expressions gaussians : 0, 2, 2. Factor e^{-ar^2} is omitted.

$\phi_{23} \rightarrow \phi_{0,3,1}$	
$\phi(\vec{r})$	y^3z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^3z$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^2z(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^3(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2yz(y^2(2a^2r^2 - 11a) + 3)$

Table 24: Orbital expressions gaussians : 0, 3, 1. Factor e^{-ar^2} is omitted.

$\phi_{24} \rightarrow \phi_{0,4,0}$	
$\phi(\vec{r})$	y^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^4$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^3(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^4z$
$\nabla^2 \phi(\vec{r})$	$2y^2(y^2(2a^2r^2 - 11a) + 6)$

Table 25: Orbital expressions gaussians : 0, 4, 0. Factor e^{-ar^2} is omitted.

$\phi_{25} \rightarrow \phi_{1,0,3}$	
$\phi(\vec{r})$	xz^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z^3(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz^3$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xz^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2xz(z^2(2a^2r^2 - 11a) + 3)$

Table 26: Orbital expressions gaussians : 1, 0, 3. Factor e^{-ar^2} is omitted.

$\phi_{26} \rightarrow \phi_{1,1,2}$	
$\phi(\vec{r})$	xyz^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$yz^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xz^2(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xyz(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy(z^2(2a^2r^2 - 11a) + 1)$

Table 27: Orbital expressions gaussians : 1, 1, 2. Factor e^{-ar^2} is omitted.

$\phi_{27} \rightarrow \phi_{1,2,1}$	
$\phi(\vec{r})$	xy^2z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^2z(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xyz(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^2(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xz(y^2(2a^2r^2 - 11a) + 1)$

Table 28: Orbital expressions gaussians : 1, 2, 1. Factor e^{-ar^2} is omitted.

$\phi_{28} \rightarrow \phi_{1,3,0}$	
$\phi(\vec{r})$	xy^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^3(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^2(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axy^3z$
$\nabla^2 \phi(\vec{r})$	$2xy(y^2(2a^2r^2 - 11a) + 3)$

Table 29: Orbital expressions gaussians : 1, 3, 0. Factor e^{-ar^2} is omitted.

$\phi_{29} \rightarrow \phi_{2,0,2}$	
$\phi(\vec{r})$	x^2z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xz^2(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz^2$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^2z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$x^2(4a^2r^2z^2 - 22az^2 + 2) + 2z^2$

Table 30: Orbital expressions gaussians : 2, 0, 2. Factor e^{-ar^2} is omitted.

$\phi_{30} \rightarrow \phi_{2,1,1}$	
$\phi(\vec{r})$	$x^2 y z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xyz (-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2 z (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2 y (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2yz (x^2 (2a^2 r^2 - 11a) + 1)$

Table 31: Orbital expressions gaussians : 2, 1, 1. Factor e^{-ar^2} is omitted.

$\phi_{31} \rightarrow \phi_{2,2,0}$	
$\phi(\vec{r})$	$x^2 y^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xy^2 (-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^2 y (-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^2 y^2 z$
$\nabla^2 \phi(\vec{r})$	$x^2 (4a^2 r^2 y^2 - 22ay^2 + 2) + 2y^2$

Table 32: Orbital expressions gaussians : 2, 2, 0. Factor e^{-ar^2} is omitted.

$\phi_{32} \rightarrow \phi_{3,0,1}$	
$\phi(\vec{r})$	$x^3 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 z (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^3 y z$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^3 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xz (x^2 (2a^2 r^2 - 11a) + 3)$

Table 33: Orbital expressions gaussians : 3, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_{33} \rightarrow \phi_{3,1,0}$	
$\phi(\vec{r})$	$x^3 y$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^3 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^3 y z$
$\nabla^2 \phi(\vec{r})$	$2xy (x^2 (2a^2 r^2 - 11a) + 3)$

Table 34: Orbital expressions gaussians : 3, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_{34} \rightarrow \phi_{4,0,0}$	
$\phi(\vec{r})$	x^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^4 y$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^4 z$
$\nabla^2 \phi(\vec{r})$	$2x^2 (x^2 (2a^2 r^2 - 11a) + 6)$

Table 35: Orbital expressions gaussians : 4, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_{35} \rightarrow \phi_{0,0,5}$	
$\phi(\vec{r})$	z^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^5$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^5$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$z^4(-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2z^3(z^2(2a^2r^2 - 13a) + 10)$

Table 36: Orbital expressions gaussians : 0, 0, 5. Factor e^{-ar^2} is omitted.

$\phi_{36} \rightarrow \phi_{0,1,4}$	
$\phi(\vec{r})$	yz^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z^4$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z^4(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2yz^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2yz^2(z^2(2a^2r^2 - 13a) + 6)$

Table 37: Orbital expressions gaussians : 0, 1, 4. Factor e^{-ar^2} is omitted.

$\phi_{37} \rightarrow \phi_{0,2,3}$	
$\phi(\vec{r})$	y^2z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2yz^3(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^2z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2z(y^2(2a^2r^2z^2 - 13az^2 + 3) + z^2)$

Table 38: Orbital expressions gaussians : 0, 2, 3. Factor e^{-ar^2} is omitted.

$\phi_{38} \rightarrow \phi_{0,3,2}$	
$\phi(\vec{r})$	y^3z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^3z^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^2z^2(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^3z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y(y^2(2a^2r^2z^2 - 13az^2 + 1) + 3z^2)$

Table 39: Orbital expressions gaussians : 0, 3, 2. Factor e^{-ar^2} is omitted.

$\phi_{39} \rightarrow \phi_{0,4,1}$	
$\phi(\vec{r})$	y^4z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^4z$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^3z(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^4(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y^2z(y^2(2a^2r^2 - 13a) + 6)$

Table 40: Orbital expressions gaussians : 0, 4, 1. Factor e^{-ar^2} is omitted.

$\phi_{40} \rightarrow \phi_{0,5,0}$	
$\phi(\vec{r})$	y^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^5$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^4(-2ay^2 + 5)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^5z$
$\nabla^2 \phi(\vec{r})$	$2y^3(y^2(2a^2r^2 - 13a) + 10)$

Table 41: Orbital expressions gaussians : 0, 5, 0. Factor e^{-ar^2} is omitted.

$\phi_{41} \rightarrow \phi_{1,0,4}$	
$\phi(\vec{r})$	xz^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z^4(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz^4$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xz^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2xz^2(z^2(2a^2r^2 - 13a) + 6)$

Table 42: Orbital expressions gaussians : 1, 0, 4. Factor e^{-ar^2} is omitted.

$\phi_{42} \rightarrow \phi_{1,1,3}$	
$\phi(\vec{r})$	xyz^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$yz^3(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xz^3(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xyz^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2xyz(z^2(2a^2r^2 - 13a) + 3)$

Table 43: Orbital expressions gaussians : 1, 1, 3. Factor e^{-ar^2} is omitted.

$\phi_{43} \rightarrow \phi_{1,2,2}$	
$\phi(\vec{r})$	xy^2z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^2z^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xyz^2(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xy^2z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x(y^2(2a^2r^2z^2 - 13az^2 + 1) + z^2)$

Table 44: Orbital expressions gaussians : 1, 2, 2. Factor e^{-ar^2} is omitted.

$\phi_{44} \rightarrow \phi_{1,3,1}$	
$\phi(\vec{r})$	xy^3z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^3z(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^2z(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^3(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xyz(y^2(2a^2r^2 - 13a) + 3)$

Table 45: Orbital expressions gaussians : 1, 3, 1. Factor e^{-ar^2} is omitted.

$\phi_{45} \rightarrow \phi_{1,4,0}$	
$\phi(\vec{r})$	xy^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^4(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xy^3(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axy^4z$
$\nabla^2 \phi(\vec{r})$	$2xy^2(y^2(2a^2r^2 - 13a) + 6)$

Table 46: Orbital expressions gaussians : 1, 4, 0. Factor e^{-ar^2} is omitted.

$\phi_{46} \rightarrow \phi_{2,0,3}$	
$\phi(\vec{r})$	x^2z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xz^3(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz^3$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2z(x^2(2a^2r^2z^2 - 13az^2 + 3) + z^2)$

Table 47: Orbital expressions gaussians : 2, 0, 3. Factor e^{-ar^2} is omitted.

$\phi_{47} \rightarrow \phi_{2,1,2}$	
$\phi(\vec{r})$	x^2yz^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xyz^2(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2z^2(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^2yz(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y(x^2(2a^2r^2z^2 - 13az^2 + 1) + z^2)$

Table 48: Orbital expressions gaussians : 2, 1, 2. Factor e^{-ar^2} is omitted.

$\phi_{48} \rightarrow \phi_{2,2,1}$	
$\phi(\vec{r})$	x^2y^2z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xy^2z(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^2yz(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2y^2(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2z(x^2(2a^2r^2y^2 - 13ay^2 + 1) + y^2)$

Table 49: Orbital expressions gaussians : 2, 2, 1. Factor e^{-ar^2} is omitted.

$\phi_{49} \rightarrow \phi_{2,3,0}$	
$\phi(\vec{r})$	x^2y^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xy^3(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2y^2(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^2y^3z$
$\nabla^2 \phi(\vec{r})$	$2y(x^2(2a^2r^2y^2 - 13ay^2 + 3) + y^2)$

Table 50: Orbital expressions gaussians : 2, 3, 0. Factor e^{-ar^2} is omitted.

$\phi_{50} \rightarrow \phi_{3,0,2}$	
$\phi(\vec{r})$	$x^3 z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 z^2 (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^3 y z^2$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^3 z (-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x (x^2 (2a^2 r^2 z^2 - 13az^2 + 1) + 3z^2)$

Table 51: Orbital expressions gaussians : 3, 0, 2. Factor e^{-ar^2} is omitted.

$\phi_{51} \rightarrow \phi_{3,1,1}$	
$\phi(\vec{r})$	$x^3 y z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y z (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^3 z (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^3 y (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xyz (x^2 (2a^2 r^2 - 13a) + 3)$

Table 52: Orbital expressions gaussians : 3, 1, 1. Factor e^{-ar^2} is omitted.

$\phi_{52} \rightarrow \phi_{3,2,0}$	
$\phi(\vec{r})$	$x^3 y^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y^2 (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^3 y (-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^3 y^2 z$
$\nabla^2 \phi(\vec{r})$	$2x (x^2 (2a^2 r^2 y^2 - 13ay^2 + 1) + 3y^2)$

Table 53: Orbital expressions gaussians : 3, 2, 0. Factor e^{-ar^2} is omitted.

$\phi_{53} \rightarrow \phi_{4,0,1}$	
$\phi(\vec{r})$	$x^4 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 z (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^4 y z$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^4 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x^2 z (x^2 (2a^2 r^2 - 13a) + 6)$

Table 54: Orbital expressions gaussians : 4, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_{54} \rightarrow \phi_{4,1,0}$	
$\phi(\vec{r})$	$x^4 y$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 y (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^4 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^4 y z$
$\nabla^2 \phi(\vec{r})$	$2x^2 y (x^2 (2a^2 r^2 - 13a) + 6)$

Table 55: Orbital expressions gaussians : 4, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_{55} \rightarrow \phi_{5,0,0}$	
$\phi(\vec{r})$	x^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^4(-2ax^2 + 5)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^5y$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^5z$
$\nabla^2 \phi(\vec{r})$	$2x^3(x^2(2a^2r^2 - 13a) + 10)$

Table 56: Orbital expressions gaussians : 5, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_{56} \rightarrow \phi_{0,0,6}$	
$\phi(\vec{r})$	z^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^6$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^6$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2z^5(-az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2z^4(z^2(2a^2r^2 - 15a) + 15)$

Table 57: Orbital expressions gaussians : 0, 0, 6. Factor e^{-ar^2} is omitted.

$\phi_{57} \rightarrow \phi_{0,1,5}$	
$\phi(\vec{r})$	yz^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axyz^5$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z^5(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$yz^4(-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2yz^3(z^2(2a^2r^2 - 15a) + 10)$

Table 58: Orbital expressions gaussians : 0, 1, 5. Factor e^{-ar^2} is omitted.

$\phi_{58} \rightarrow \phi_{0,2,4}$	
$\phi(\vec{r})$	y^2z^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z^4$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2yz^4(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^2z^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2z^2(y^2(2a^2r^2z^2 - 15az^2 + 6) + z^2)$

Table 59: Orbital expressions gaussians : 0, 2, 4. Factor e^{-ar^2} is omitted.

$\phi_{59} \rightarrow \phi_{0,3,3}$	
$\phi(\vec{r})$	y^3z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^3z^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^2z^3(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^3z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2yz(y^2(2a^2r^2z^2 - 15az^2 + 3) + 3z^2)$

Table 60: Orbital expressions gaussians : 0, 3, 3. Factor e^{-ar^2} is omitted.

$\phi_{60} \rightarrow \phi_{0,4,2}$	
$\phi(\vec{r})$	$y^4 z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^4 z^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^3 z^2 (-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^4 z (-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y^2 (y^2 (2a^2 r^2 z^2 - 15az^2 + 1) + 6z^2)$

Table 61: Orbital expressions gaussians : 0, 4, 2. Factor e^{-ar^2} is omitted.

$\phi_{61} \rightarrow \phi_{0,5,1}$	
$\phi(\vec{r})$	$y^5 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^5 z$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^4 z (-2ay^2 + 5)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^5 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y^3 z (y^2 (2a^2 r^2 - 15a) + 10)$

Table 62: Orbital expressions gaussians : 0, 5, 1. Factor e^{-ar^2} is omitted.

$\phi_{62} \rightarrow \phi_{0,6,0}$	
$\phi(\vec{r})$	y^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^6$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^5 (-ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^6 z$
$\nabla^2 \phi(\vec{r})$	$2y^4 (y^2 (2a^2 r^2 - 15a) + 15)$

Table 63: Orbital expressions gaussians : 0, 6, 0. Factor e^{-ar^2} is omitted.

$\phi_{63} \rightarrow \phi_{1,0,5}$	
$\phi(\vec{r})$	xz^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z^5 (-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz^5$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xz^4 (-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2xz^3 (z^2 (2a^2 r^2 - 15a) + 10)$

Table 64: Orbital expressions gaussians : 1, 0, 5. Factor e^{-ar^2} is omitted.

$\phi_{64} \rightarrow \phi_{1,1,4}$	
$\phi(\vec{r})$	xyz^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$yz^4 (-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xz^4 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xyz^3 (-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2xyz^2 (z^2 (2a^2 r^2 - 15a) + 6)$

Table 65: Orbital expressions gaussians : 1, 1, 4. Factor e^{-ar^2} is omitted.

$\phi_{65} \rightarrow \phi_{1,2,3}$	
$\phi(\vec{r})$	xy^2z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^2z^3(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xyz^3(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^2z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2xz(y^2(2a^2r^2z^2 - 15az^2 + 3) + z^2)$

Table 66: Orbital expressions gaussians : 1, 2, 3. Factor e^{-ar^2} is omitted.

$\phi_{66} \rightarrow \phi_{1,3,2}$	
$\phi(\vec{r})$	xy^3z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^3z^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^2z^2(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xy^3z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy(y^2(2a^2r^2z^2 - 15az^2 + 1) + 3z^2)$

Table 67: Orbital expressions gaussians : 1, 3, 2. Factor e^{-ar^2} is omitted.

$\phi_{67} \rightarrow \phi_{1,4,1}$	
$\phi(\vec{r})$	xy^4z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^4z(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xy^3z(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^4(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy^2z(y^2(2a^2r^2 - 15a) + 6)$

Table 68: Orbital expressions gaussians : 1, 4, 1. Factor e^{-ar^2} is omitted.

$\phi_{68} \rightarrow \phi_{1,5,0}$	
$\phi(\vec{r})$	xy^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^5(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^4(-2ay^2 + 5)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axy^5z$
$\nabla^2 \phi(\vec{r})$	$2xy^3(y^2(2a^2r^2 - 15a) + 10)$

Table 69: Orbital expressions gaussians : 1, 5, 0. Factor e^{-ar^2} is omitted.

$\phi_{69} \rightarrow \phi_{2,0,4}$	
$\phi(\vec{r})$	x^2z^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xz^4(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz^4$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^2z^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2z^2(x^2(2a^2r^2z^2 - 15az^2 + 6) + z^2)$

Table 70: Orbital expressions gaussians : 2, 0, 4. Factor e^{-ar^2} is omitted.

$\phi_{70} \rightarrow \phi_{2,1,3}$	
$\phi(\vec{r})$	$x^2 y z^3$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x y z^3 (-a x^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2 z^3 (-2a y^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2 y z^2 (-2a z^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2y z (x^2 (2a^2 r^2 z^2 - 15a z^2 + 3) + z^2)$

Table 71: Orbital expressions gaussians : 2, 1, 3. Factor e^{-ar^2} is omitted.

$\phi_{71} \rightarrow \phi_{2,2,2}$	
$\phi(\vec{r})$	$x^2 y^2 z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x y^2 z^2 (-a x^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^2 y z^2 (-a y^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^2 y^2 z (-a z^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$x^2 (4a^2 r^2 y^2 z^2 - 30a y^2 z^2 + 2y^2 + 2z^2) + 2y^2 z^2$

Table 72: Orbital expressions gaussians : 2, 2, 2. Factor e^{-ar^2} is omitted.

$\phi_{72} \rightarrow \phi_{2,3,1}$	
$\phi(\vec{r})$	$x^2 y^3 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x y^3 z (-a x^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^2 y^2 z (-2a y^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2 y^3 (-2a z^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y z (x^2 (2a^2 r^2 y^2 - 15a y^2 + 3) + y^2)$

Table 73: Orbital expressions gaussians : 2, 3, 1. Factor e^{-ar^2} is omitted.

$\phi_{73} \rightarrow \phi_{2,4,0}$	
$\phi(\vec{r})$	$x^2 y^4$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x y^4 (-a x^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^2 y^3 (-a y^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2a x^2 y^4 z$
$\nabla^2 \phi(\vec{r})$	$2y^2 (x^2 (2a^2 r^2 y^2 - 15a y^2 + 6) + y^2)$

Table 74: Orbital expressions gaussians : 2, 4, 0. Factor e^{-ar^2} is omitted.

$\phi_{74} \rightarrow \phi_{3,0,3}$	
$\phi(\vec{r})$	$x^3 z^3$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 z^3 (-2a x^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2a x^3 y z^3$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^3 z^2 (-2a z^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2x z (x^2 (2a^2 r^2 z^2 - 15a z^2 + 3) + 3z^2)$

Table 75: Orbital expressions gaussians : 3, 0, 3. Factor e^{-ar^2} is omitted.

$\phi_{75} \rightarrow \phi_{3,1,2}$	
$\phi(\vec{r})$	$x^3 y z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y z^2 (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^3 z^2 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^3 y z (-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy (x^2 (2a^2 r^2 z^2 - 15az^2 + 1) + 3z^2)$

Table 76: Orbital expressions gaussians : 3, 1, 2. Factor e^{-ar^2} is omitted.

$\phi_{76} \rightarrow \phi_{3,2,1}$	
$\phi(\vec{r})$	$x^3 y^2 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y^2 z (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^3 y z (-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^3 y^2 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xz (x^2 (2a^2 r^2 y^2 - 15ay^2 + 1) + 3y^2)$

Table 77: Orbital expressions gaussians : 3, 2, 1. Factor e^{-ar^2} is omitted.

$\phi_{77} \rightarrow \phi_{3,3,0}$	
$\phi(\vec{r})$	$x^3 y^3$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^2 y^3 (-2ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^3 y^2 (-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^3 y^3 z$
$\nabla^2 \phi(\vec{r})$	$2xy (x^2 (2a^2 r^2 y^2 - 15ay^2 + 3) + 3y^2)$

Table 78: Orbital expressions gaussians : 3, 3, 0. Factor e^{-ar^2} is omitted.

$\phi_{78} \rightarrow \phi_{4,0,2}$	
$\phi(\vec{r})$	$x^4 z^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 z^2 (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^4 y z^2$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2x^4 z (-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x^2 (x^2 (2a^2 r^2 z^2 - 15az^2 + 1) + 6z^2)$

Table 79: Orbital expressions gaussians : 4, 0, 2. Factor e^{-ar^2} is omitted.

$\phi_{79} \rightarrow \phi_{4,1,1}$	
$\phi(\vec{r})$	$x^4 y z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 y z (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^4 z (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^4 y (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x^2 y z (x^2 (2a^2 r^2 - 15a) + 6)$

Table 80: Orbital expressions gaussians : 4, 1, 1. Factor e^{-ar^2} is omitted.

$\phi_{80} \rightarrow \phi_{4,2,0}$	
$\phi(\vec{r})$	$x^4 y^2$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^3 y^2 (-ax^2 + 2)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2x^4 y (-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^4 y^2 z$
$\nabla^2 \phi(\vec{r})$	$2x^2 (x^2 (2a^2 r^2 y^2 - 15ay^2 + 1) + 6y^2)$

Table 81: Orbital expressions gaussians : 4, 2, 0. Factor e^{-ar^2} is omitted.

$\phi_{81} \rightarrow \phi_{5,0,1}$	
$\phi(\vec{r})$	$x^5 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^4 z (-2ax^2 + 5)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^5 y z$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^5 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2x^3 z (x^2 (2a^2 r^2 - 15a) + 10)$

Table 82: Orbital expressions gaussians : 5, 0, 1. Factor e^{-ar^2} is omitted.

$\phi_{82} \rightarrow \phi_{5,1,0}$	
$\phi(\vec{r})$	$x^5 y$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$x^4 y (-2ax^2 + 5)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$x^5 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^5 y z$
$\nabla^2 \phi(\vec{r})$	$2x^3 y (x^2 (2a^2 r^2 - 15a) + 10)$

Table 83: Orbital expressions gaussians : 5, 1, 0. Factor e^{-ar^2} is omitted.

$\phi_{83} \rightarrow \phi_{6,0,0}$	
$\phi(\vec{r})$	x^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2x^5 (-ax^2 + 3)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^6 y$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ax^6 z$
$\nabla^2 \phi(\vec{r})$	$2x^4 (x^2 (2a^2 r^2 - 15a) + 15)$

Table 84: Orbital expressions gaussians : 6, 0, 0. Factor e^{-ar^2} is omitted.

$\phi_{84} \rightarrow \phi_{0,0,7}$	
$\phi(\vec{r})$	z^7
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axz^7$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ayz^7$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$z^6 (-2az^2 + 7)$
$\nabla^2 \phi(\vec{r})$	$2z^5 (z^2 (2a^2 r^2 - 17a) + 21)$

Table 85: Orbital expressions gaussians : 0, 0, 7. Factor e^{-ar^2} is omitted.

$\phi_{85} \rightarrow \phi_{0,1,6}$	
$\phi(\vec{r})$	yz^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axyz^6$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$z^6(-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2yz^5(-az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2yz^4(z^2(2a^2r^2 - 17a) + 15)$

Table 86: Orbital expressions gaussians : 0, 1, 6. Factor e^{-ar^2} is omitted.

$\phi_{86} \rightarrow \phi_{0,2,5}$	
$\phi(\vec{r})$	y^2z^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^2z^5$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2yz^5(-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^2z^4(-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2z^3(y^2(2a^2r^2z^2 - 17az^2 + 10) + z^2)$

Table 87: Orbital expressions gaussians : 0, 2, 5. Factor e^{-ar^2} is omitted.

$\phi_{87} \rightarrow \phi_{0,3,4}$	
$\phi(\vec{r})$	y^3z^4
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^3z^4$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^2z^4(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^3z^3(-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2yz^2(y^2(2a^2r^2z^2 - 17az^2 + 6) + 3z^2)$

Table 88: Orbital expressions gaussians : 0, 3, 4. Factor e^{-ar^2} is omitted.

$\phi_{88} \rightarrow \phi_{0,4,3}$	
$\phi(\vec{r})$	y^4z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^4z^3$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^3z^3(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^4z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2y^2z(y^2(2a^2r^2z^2 - 17az^2 + 3) + 6z^2)$

Table 89: Orbital expressions gaussians : 0, 4, 3. Factor e^{-ar^2} is omitted.

$\phi_{89} \rightarrow \phi_{0,5,2}$	
$\phi(\vec{r})$	y^5z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^5z^2$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^4z^2(-2ay^2 + 5)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2y^5z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y^3(y^2(2a^2r^2z^2 - 17az^2 + 1) + 10z^2)$

Table 90: Orbital expressions gaussians : 0, 5, 2. Factor e^{-ar^2} is omitted.

$\phi_{90} \rightarrow \phi_{0,6,1}$	
$\phi(\vec{r})$	$y^6 z$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^6 z$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2y^5 z (-ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$y^6 (-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2y^4 z (y^2 (2a^2 r^2 - 17a) + 15)$

Table 91: Orbital expressions gaussians : 0, 6, 1. Factor e^{-ar^2} is omitted.

$\phi_{91} \rightarrow \phi_{0,7,0}$	
$\phi(\vec{r})$	y^7
$\vec{i} \cdot \nabla \phi(\vec{r})$	$-2axy^7$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$y^6 (-2ay^2 + 7)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2ay^7 z$
$\nabla^2 \phi(\vec{r})$	$2y^5 (y^2 (2a^2 r^2 - 17a) + 21)$

Table 92: Orbital expressions gaussians : 0, 7, 0. Factor e^{-ar^2} is omitted.

$\phi_{92} \rightarrow \phi_{1,0,6}$	
$\phi(\vec{r})$	xz^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$z^6 (-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2axyz^6$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xz^5 (-az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2xz^4 (z^2 (2a^2 r^2 - 17a) + 15)$

Table 93: Orbital expressions gaussians : 1, 0, 6. Factor e^{-ar^2} is omitted.

$\phi_{93} \rightarrow \phi_{1,1,5}$	
$\phi(\vec{r})$	xyz^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$yz^5 (-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xz^5 (-2ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xyz^4 (-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2xyz^3 (z^2 (2a^2 r^2 - 17a) + 10)$

Table 94: Orbital expressions gaussians : 1, 1, 5. Factor e^{-ar^2} is omitted.

$\phi_{94} \rightarrow \phi_{1,2,4}$	
$\phi(\vec{r})$	$xy^2 z^4$
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^2 z^4 (-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xyz^4 (-ay^2 + 1)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xy^2 z^3 (-az^2 + 2)$
$\nabla^2 \phi(\vec{r})$	$2xz^2 (y^2 (2a^2 r^2 z^2 - 17az^2 + 6) + z^2)$

Table 95: Orbital expressions gaussians : 1, 2, 4. Factor e^{-ar^2} is omitted.

$\phi_{95} \rightarrow \phi_{1,3,3}$	
$\phi(\vec{r})$	xy^3z^3
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^3z^3(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^2z^3(-2ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^3z^2(-2az^2 + 3)$
$\nabla^2 \phi(\vec{r})$	$2xyz(y^2(2a^2r^2z^2 - 17az^2 + 3) + 3z^2)$

Table 96: Orbital expressions gaussians : 1, 3, 3. Factor e^{-ar^2} is omitted.

$\phi_{96} \rightarrow \phi_{1,4,2}$	
$\phi(\vec{r})$	xy^4z^2
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^4z^2(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xy^3z^2(-ay^2 + 2)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$2xy^4z(-az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy^2(y^2(2a^2r^2z^2 - 17az^2 + 1) + 6z^2)$

Table 97: Orbital expressions gaussians : 1, 4, 2. Factor e^{-ar^2} is omitted.

$\phi_{97} \rightarrow \phi_{1,5,1}$	
$\phi(\vec{r})$	xy^5z
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^5z(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$xy^4z(-2ay^2 + 5)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$xy^5(-2az^2 + 1)$
$\nabla^2 \phi(\vec{r})$	$2xy^3z(y^2(2a^2r^2 - 17a) + 10)$

Table 98: Orbital expressions gaussians : 1, 5, 1. Factor e^{-ar^2} is omitted.

$\phi_{98} \rightarrow \phi_{1,6,0}$	
$\phi(\vec{r})$	xy^6
$\vec{i} \cdot \nabla \phi(\vec{r})$	$y^6(-2ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$2xy^5(-ay^2 + 3)$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$-2axy^6z$
$\nabla^2 \phi(\vec{r})$	$2xy^4(y^2(2a^2r^2 - 17a) + 15)$

Table 99: Orbital expressions gaussians : 1, 6, 0. Factor e^{-ar^2} is omitted.

$\phi_{99} \rightarrow \phi_{2,0,5}$	
$\phi(\vec{r})$	x^2z^5
$\vec{i} \cdot \nabla \phi(\vec{r})$	$2xz^5(-ax^2 + 1)$
$\vec{j} \cdot \nabla \phi(\vec{r})$	$-2ax^2yz^5$
$\vec{k} \cdot \nabla \phi(\vec{r})$	$x^2z^4(-2az^2 + 5)$
$\nabla^2 \phi(\vec{r})$	$2z^3(x^2(2a^2r^2z^2 - 17az^2 + 10) + z^2)$

Table 100: Orbital expressions gaussians : 2, 0, 5. Factor e^{-ar^2} is omitted.