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Understanding Atomic (Hydrogenic) Hybrid Orbitals Part 2, $sp^2$

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I. SYNOPSIS

This is a continuation of the discussion of hybrid orbitals, this time focusing on $sp^2$ orbitals, the last of the sets which can be plotted easily on a piece of paper.

II. INTRODUCTION

We here address them with $sp^2$ orbitals. They are combinations of a $2s$ orbital and two $2p$ orbitals, $2p_x$ and $2p_y$. The $2p_z$ orbital is normally reserved for use in $\pi$ bonding, which is another topic.

III. NORMALIZATION

We show, in the attached Maple code, that the normalization constants for the $2s$ and $2p$ orbitals that contribute herein are the same, and therefore ignorable (from our point of view of plotting them).

IV. $sp^2$ ORBITALS

We start with an $s$ and two $p$ orbitals. The standard choice involves using $p_x$ and $p_y$ orbitals. We arbitrarily choose to keep the $p_z$ orbital by itself (often used to form $\pi$ bonds, but that’s another story) [1].

$$
\psi_{sp^2_1} = \frac{1}{\sqrt{3}} \psi_{2s} + \sqrt{\frac{2}{3}} \psi_{2p_x} + 0 \psi_{2p_y}
$$

and

$$
\psi_{sp^2_2} = \frac{1}{\sqrt{3}} \psi_{2s} - \frac{1}{\sqrt{6}} \psi_{2p_x} + \frac{1}{\sqrt{2}} \psi_{2p_y}
$$

Note that we do not use a $1s$ orbital! The $2s$ hydrogenic orbital has the form

$$
\psi_{2s} = (2 - r)e^{-r/2}
$$

where we are still assuming an atomic charge of 1 (we could assume a carbon like value, but would learn almost nothing from it, so why bother?). The $p_z$ orbital has the form

$$
\psi_{2p_z} = r \sin \theta \cos \varphi e^{-r/2}
$$

as usual.

In Cartesian coordinates we have

$$
\psi_{sp^2} = \left(2 - \sqrt{x^2 + y^2 + z^2}\right) e^{\sqrt{x^2+y^2+z^2}/2}
$$

How are we to understand this orbital, as given?

V. A NON-TRADITIONAL PLOT

Let’s do what we did with simple hydrogenic orbitals, i.e., plot $\psi_{sp^2}(x,0,z)$ versus $x$ and $z$. We see that there is a positive peak somewhere in the region $z > 0$. There is a valley (negative) appearing on the negative $z$ axis. Both of these features tail off as $|x|$ grows.

VI. A CONTOUR PLOT

We next create a contour plot of $\psi_{sp^2}(x,y,0)$ versus $x$ and $y$ in two dimensions. This is Figure 2, a plot showing loci of constant $\psi$.

Typeset by REVTeX
FIG. 2: A contour map of $\psi(x, y, 0)$ with $x$ and $y$

VII. NON-TRADITIONAL PLOTS

Now, we want to look a little more at this function. First, we re-write it as

$$\psi_{sp^2} = ((2 - r) + r \sin \theta \cos \varphi) e^{r/2}$$

and fix the value of $r$ at some (arbitrary) value, say “1”. Then, ignoring the exponential, we have

$$\psi_{sp^2} = ((2 - 1) + 1 \sin \theta \cos \varphi) e^{r/2}$$

and we now set $\vartheta = \frac{\pi}{2}$ so that we are “in the $x$-$y$ plane. this allows us to make a polar plot of this function $(1 + \cos \varphi)$ in the traditional manner. We eschew this here, since we’ve done it before for the $sp$ case.

Instead, we construct the 3-dimensional contour plot in $x$, $y$, and $z$ space in Figure 3. Notice that this is really two plots, one for the positive lobe, the other for the negative one, superimposed.

VIII. ANOTHER $sp^2$ ORBITAL

We will see here that the next $sp^2$ orbital is canted relative to the first one we drew. Actually, as shown in some texts, they are 120$^\circ$ apart, as is the last one. Thus the trigonal structure of $sp^2$ central atom bonding is established.

Figure 4 shows the $\psi_{sp^2}(x, y, 0)$ versus $x$ and $y$, while Figures 5 and 6 show the contour map and contour surface, respectively of this canted orbital.

IX. MAPLE

To help in this learning, perhaps the following code will be found useful.

```maple
> #sp2-hybrid-plot
> restart;
> with(plots);
> fs := exp(-r/2);
> psi_2s := (2-r)*fs;
> cart_psi_2p_x := x*fs;
> cart_psi_2p_y := y*fs;
> cart_psi_2p_z := z*fs;
> psi_2p_x := r*sin(theta)*cos(phi)*fs;
> psi_2p_y := r*sin(theta)*sin(phi)*fs;
> psi_2p_z := r*cos(theta)*fs;
> t11 := int(r^2*sin(theta)*psi_2p_x^2,phi=0..2*Pi):
> t21 := int(t11,theta=0..Pi):
> t31 := int(t21,r=0..infinity):
> N_2px := sqrt(t31);
> t12 := int(r^2*sin(theta)*psi_2s^2,phi=0..2*Pi):
> t22 := int(t12,theta=0..Pi):
> t32 := int(t22,r=0..infinity):
> N_2s := sqrt(t32);
> print ('the normalization constants are the same, so we can ignore them');
Warning, the name changecoords has been redefined
```
FIG. 3: $\psi = constant$ contour 3D plot. This is a composite, with the positive and negative lobes colored differently.

FIG. 4: Similar to the first $sp^2$ orbital, but pointing elsewhere. Again, notice the captioning error.

[animate, animate3d, animatecurve, arrow, changecoords, complexplot, complexplot3d, conformal, conformal3d, contourplot, contourplot3d, coordplot, coordplot3d, cylinderplot, densityplot, display, display3d, fieldplot, fieldplot3d, gradplot, gradplot3d, graphplot3d, implicitplot, implicitplot3d, inequal, interactive, listcontplot, listcontplot3d, listdensityplot, listplot, listplot3d, loglogplot, logplot, matrixplot, odeplot, pareto, plotcompare, pointplot, pointplot3d, polarplot, polygonplot, polygonplot3d, polyhedra, polyhedra_supported, polyhedrplot, replot, roolocplot, semilogplot, setoptions, setoptions3d, spacecurve, sparsematrixplot, sphereplot, surfdata, textplot, textplot3d, tubeplot]

\[
fs := e^{-r^2}
\]

\[
psi_2s := (2 - r)e^{-r^2}
\]

\[
cart_psi_2p_x := x e^{-r^2}
\]

\[
cart_psi_2p_y := y e^{-r^2}
\]
FIG. 5: The contour map of the second $sp^2$ orbital.

FIG. 6: The pseudo 3D implicitplot03D surface of $\psi(x, y, z)$ versus $x$, $y$, and $z$. This is a composite of the two lobes, one positive, one negative.

\[
cart_{\text{psi}_z} := z e^{-\frac{x^2}{2}}
\]
\[
\psi_{2p,x} := r \sin(\theta) \cos(\phi) e^{-\frac{r^2}{2}}
\]
\[
\psi_{2p,y} := r \sin(\theta) \sin(\phi) e^{-\frac{r^2}{2}}
\]
\[
\psi_{2p,z} := r \cos(\theta) e^{-\frac{r^2}{2}}
\]
\[
N_{2p} := 4 \sqrt{2} \sqrt{\pi}
\]
\[
N_{2s} := 4 \sqrt{2} \sqrt{\pi}
\]

The normalization constants are the same, so we can ignore them.
#note, un-normalized orbitals in use!
r := sqrt(x^2+y^2+z^2):
t1 := ((1/sqrt(3))*psi_2s+(sqrt(2/3))*cart_psi_2p_x);#page 372 Karplus & Porter
lim := 4;
plot3d(subs(z=0,t1),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x','y',
',psi'],title='2sp^2(x,y,0) versus x and z');
contourplot(subs(z=0,t1),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x
',',y'],title='2sp^2 hybrid orbital contour plot ',contours = 20);
lim := 8;
f1 := implicitplot3d(t1=0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED,
labels=['x','y','z'],color=blue):
f2 := implicitplot3d(t1=-0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED
,labels=['x','y','z'],title='2sp^2 hybrid orbital (composite +(blue)
and -(red))',color=red):
display(f1,f2);
#============================================
t2 := ((1/sqrt(3))*psi_2s-(sqrt(1/6))*cart_psi_2p_x+
+(1/sqrt(2))*cart_psi_2p_y);#page 372 Karplus & Porter
lim := 4;
plot3d(subs(z=0,t2),x=-lim..lim,y=-lim..lim,axes=BOXED,labels=['x','y','z'],title='2sp^2 hybrid orbital contour plot ',contours = 20);
lim := 8;
f1 := implicitplot3d(t2=0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED,
labels=['x','y','z'],color=blue):
f2 := implicitplot3d(t2=-0.08,x=-lim..lim,y=-lim..lim,z=-lim..lim,axes=BOXED
,labels=['x','y','z'],title='2sp^2 hybrid orbital (composite +(blue)
and -(red))',color=red):
display(f1,f2);

\[ t_1 := \frac{1}{3} \sqrt{3} (2 - \sqrt{x^2 + y^2 + z^2}) e^{(-\frac{x^2+y^2+z^2}{\sqrt{2}})} + \frac{1}{3} \sqrt{6} x e^{(-\frac{x^2+y^2+z^2}{\sqrt{2}})} \]
\[ \text{lim} := 4 \]
\[ \text{lim} := 8 \]

\[ t_2 := \frac{1}{3} \sqrt{3} (2 - \sqrt{x^2 + y^2 + z^2}) e^{(-\frac{x^2+y^2+z^2}{\sqrt{2}})} - \frac{1}{6} \sqrt{6} x e^{(-\frac{x^2+y^2+z^2}{\sqrt{2}})} + \frac{1}{2} \sqrt{2} y e^{(-\frac{x^2+y^2+z^2}{\sqrt{2}})} \]
\[ \%1 := x^2 + y^2 + z^2 \]
\[ \text{lim} := 4 \]
\[ \text{lim} := 8 \]