# Atomic Orbitals and Hybridization

#### Using the Hybridization Lab Tool

Locate the following buttons:

Hybridize p <sub>x</sub> Hybridize p <sub>y</sub> Hybridiz	ze p <sub>z</sub> Hide Unhybridized p Orbitals	Reset
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The "Hybridize" buttons can be used to control which p orbitals are entered into hybridization. The s orbital is always used, so it is locked to the *on* position.

"Hide Unhybridized P Orbitals" allows you to more easily see the hybrid orbitals by making the larger, visually obstructive p orbitals invisible. You may find this useful when sketching the hybrid orbitals.

"Reset" returns the system to its original state, removing all orbitals from hybridization.

#### **Part I: Atomic Orbitals**

Examine the set of s and p orbitals shown along the top of the screen, and in the "Atomic Shape" box where they can all be seen superimposed. Note how the orbitals are oriented in space, and sketch them each individually below.

p orbital	p orbital	p orbital	s orbital

- How many orbitals are in this set?
- What is the angle between the *different* p orbitals?

### Part II: sp Hybridization

Press *Hybridize*  $p_x$ . The s orbital and one of the p orbitals will disappear, to be replaced with **two** new hybrid orbitals. (Unlike the p orbitals, each lobe here is a separate orbital.)

Press *Hide Unhybridized p Orbitals,* to get a better look at the hybrid orbitals. Sketch them here, along with the now-modified energy level diagram.

#### sp Hybrid Orbitals

• What is the angle between the hybrid orbitals?

Now, click *Show Unhybridized p Orbitals*. Note where they are, relative to the hybrid orbitals.

- How many p orbitals remain?
- How many hybrid orbitals are there?
- In all, how many orbitals are in this set? (Hybrid plus p orbitals)

Press *Reset,* and repeat the process for the other two p orbitals. Keep track of the differences (if any) and draw them and their associated energy level diagrams below.

Other sp Hybrid Orbitals

s+py

s+p<sub>x</sub>

s+p<sub>z</sub>

• What are the angles between the other sp hybrid orbitals?

## Part III: sp<sup>2</sup> Hybridization

After resetting the system, press *Hybridize*  $p_x$  and then *Hybridize*  $p_z$ . Press *Hide Unhybridized* p *Orbitals*, and then note the number and direction of the new hybrids. Also, notice the new energy level diagram. Sketch the hybrid orbitals below.

sp <sup>2</sup> Hybrid Orbitals
s+p <sub>x</sub> +p <sub>z</sub>

• What are the angles between the hybrid orbitals?

Click *Show Unhybridized p Orbitals,* and look at where the remaining p orbital is.

• How many p orbitals remain?

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- How many hybrid orbitals are there?
- In all, how many orbitals are in this set? (Hybrid plus p orbitals)

Press *Reset* and then repeat the process for the other two-orbital combinations. Keep track of the differences (if any) and draw them and their associated energy level diagrams below.

# Other sp<sup>2</sup> Hybrid Orbitals s+p<sub>x</sub>+p<sub>y</sub> s+p<sub>y</sub>+p<sub>z</sub>

What are the angles between the other sp<sup>2</sup> hybrid orbitals?

## Part IV: sp<sup>3</sup> Hybridization

Reset the system and press all three *Hybridize* buttons. Sketch the hybrid orbitals and their energy levels below.

sp <sup>3</sup> Hybrid Orbitals	
	$s+p_x+p_y+p_z$

- What is the angle between the hybrid orbitals?
- Are there any p orbitals left?
- How many hybrid orbitals are there?
- In all, how many orbitals are in this set? (Hybrid plus p orbitals)

#### Part V: Follow-up Questions

**1)** Describe the bonding in BeCl<sub>2</sub>, BF<sub>3</sub>, CH<sub>4</sub>, and NH<sub>3</sub> using the localized electron model. This will involve three steps:

- Write the "best" Lewis Structures.
- Use VSEPR to determine the arrangement of the electron pairs.
- Determine the hybrid atomic orbitals involved.

**2)** For each molecule above, sketch the associated orbital energy levels for the central atom.