1. The sp hybrid orbital defined below has the correct ratio of $(2s)$ and $(2p_z)$ but is not yet normalized. Find the normalization constant A_a, and then write the expression for the normalized hybrid orbital $(sp)_b$ that accompanies $(sp)_a$.

$$(sp)_a = A_a \left[(2s) + \frac{1}{\sqrt{3}}(2p_z) \right]$$

$$\int (sp)_a^2 \, d\tau = A_a^2 \left[1 + \frac{1}{3} \right] = \frac{4}{3} A_a = 1$$

$$\boxed{A_a = \pm\sqrt{\frac{3}{4}}}$$

$$(sp)_a = \sqrt{\frac{3}{4}}(2s) + \sqrt{\frac{1}{4}}(2p_z)$$

$$(sp)_b = b(2s) + c(2p_z)$$

$$0 = \sqrt{\frac{3}{4}}b + \sqrt{\frac{1}{4}}c \quad \text{if } (sp)_a \text{ and } (sp)_b \text{ orthogonal}$$

$$c = -\sqrt{3}b$$

$$1 = b^2 + c^2 \quad \text{if } (sp)_b \text{ normalized}$$

$$= b^2 + (-\sqrt{3}b)^2 = 4b^2$$

$$b = \pm\sqrt{\frac{1}{4}} = \pm\frac{1}{2}$$

$$(sp)_b = \frac{1}{2}(2s) - \sqrt{\frac{3}{4}}(2p_z)$$

2. Write the name of the *smallest* point group that contains the operators $\hat{C}_5$ and $\hat{I}$.
   Solution: You can solve this different ways. The most methodical way would be to start with these two operators and their products to see what other operators must be in the group. Clearly we need $\hat{I}^2 = \hat{E}$, and all the successive $\hat{C}_5$ rotations: $\hat{C}_5^2$, $\hat{C}_5^3$, $\hat{C}_5^4$. But what about $\hat{I}\hat{C}_5$? If the $\hat{C}_5$ is rotation about the z axis by $2\pi/5$, then $\hat{I}\hat{C}_5$ is a rotation by $\pi + (2\pi/5) = 7\pi/5 = 7(2\pi/10)$, followed by reflection through the xy plane. That's equivalent to the operation $\hat{\sigma}_h\hat{C}_{10}^7 = \hat{S}_{10}^7$. Any other combination of $\hat{I}$ and $\hat{C}_5^n$ will yield some $\hat{S}_{10}^m$. Therefore, we need the group with $\hat{E}$, $4\hat{C}_5$, $\hat{I}$, and four $\hat{S}_{10}$ operators: $\hat{S}_{10}$, $\hat{S}_{10}^3$, $\hat{S}_{10}^7$, $\hat{S}_{10}^9$. (Any even power of $\hat{S}_n$ is a proper rotation, and $\hat{S}_{10}^5$ is the same as $\hat{\sigma}_h\hat{C}_2 = \hat{I}$.) This group is $\boxed{S_{10}}$. It has 10 operators. Other small-ish groups with $\hat{C}_5$ and $\hat{I}$ are C_{10h} (20 operators) and D_{5d} (20 operators).

3. Find the point group of this hexahydroxybenzene. This conformation is planar.
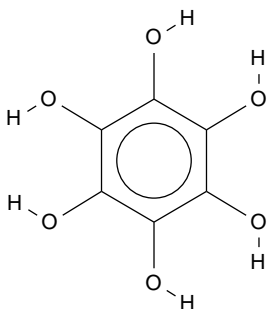
D_{3h}

4. Fill in the phases for the p orbitals in (c) and label the coordinates on the Cartesian axes to obtain a new molecular orbital for 1,4-hexadiene that has b_{3g} symmetry. **Solution:** The point group is D_{2h}. According to that character table, the representation b_{1u} must be antisymmetric under $\hat{\sigma}(xy)$, so that must be the plane of the molecule. This doesn't specify which axis is x and which is y, however, so there are two possible solutions to the problem. The b_{3g} MO must be symmetric under $\hat{\sigma}(xz)$ and antisymmetric under $\hat{\sigma}(yz)$.
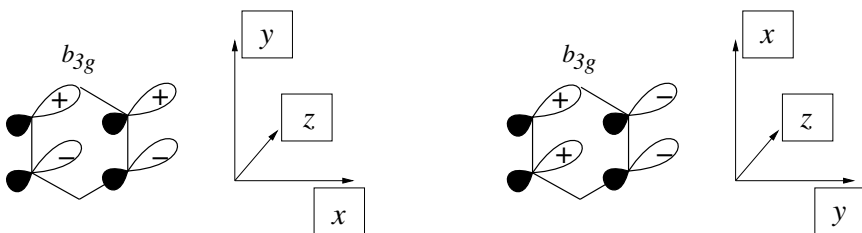
5. Find the symmetry representations of all of the states accessible by an *allowed Raman transition* from the B_{1u} excited state of benzene.

Solution: the point group is D_{6h}, and we need the final state representations Γ to be those that yield Γ_μ equal to any of A_{1g}, E_{1g}, or E_{2g}, the representations for the Raman operators.

D_{6h}	$\hat{E}$	$2\hat{C}_6$	$2\hat{C}_3$	$\hat{C}_2$	$\hat{I}$	
B_{1u}	1	-1	1	-1	-1	
A_{1g}	1	1	1	1	1	
A_{1g}/B_{1u}	1	-1	1	-1	-1	$= \boxed{B_{1u}}$
E_{1g}	2	1	-1	-2	2	
E_{1g}/B_{1u}	2	-1	-1	2	-2	$= \boxed{E_{2u}}$
E_{2g}	2	-1	-1	2	2	
E_{2g}/B_{1u}	2	1	-1	-2	-2	$= \boxed{E_{1u}}$