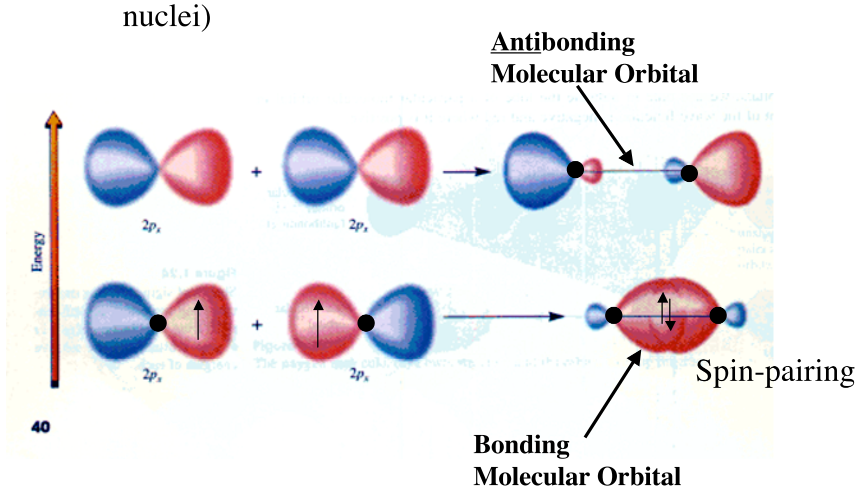
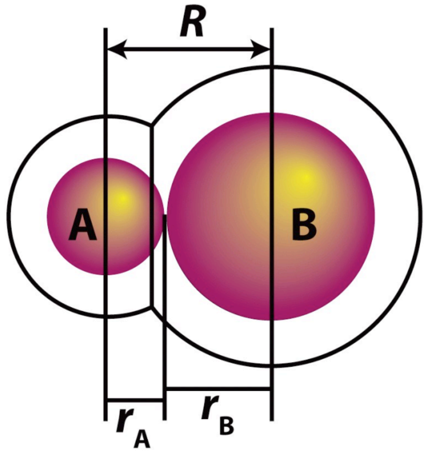
Using Symmetry to Generate Molecular Orbital Diagrams

- review a few MO concepts
- generate MO for XH_2, H_2O, SF_6

Formation of a bond occurs when electron density collects between the two bonded nuclei (ie., Ψ^2_{MO}= large in the region of space between nuclei)



……. the valence electrons draw the atoms together until the core electrons start to repel one other, and that dominates



10 Covalent radius

Structure 2-10
Shriver & Atkins Inorganic Chemistry, Fourth Edition

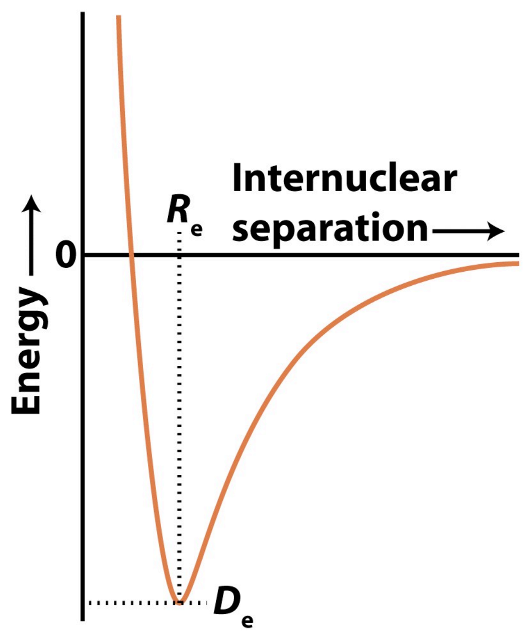


Figure 2-5
Shriver & Atkins Inorganic Chemistry, Fourth Edition

the total number of molecular orbitals (MO's) generated= total number of atomic orbitals (AO's) combined

Atom A + Atom B
(4 AO's) (4 AO's)

Molecule A–B
(8 MO's)

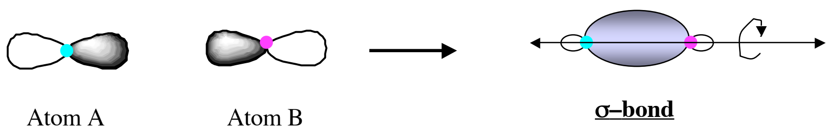
in order to overlap……...

Atom A + Atom B
(4 AO's) (4 AO's)

AO's must have:

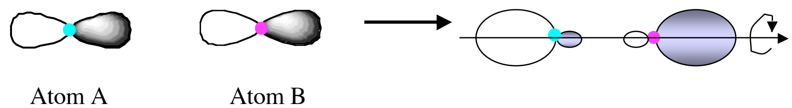
- **similar energies**
- **identical symmetries**

Molecule A–B
(8 MO's)



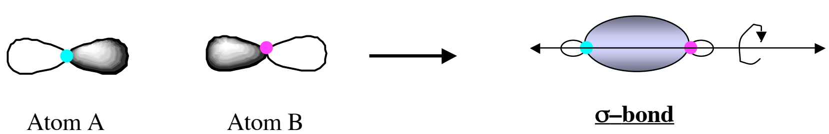
<u>σ–bond</u>

doesn't change sign
upon rotation about
internuclear axis



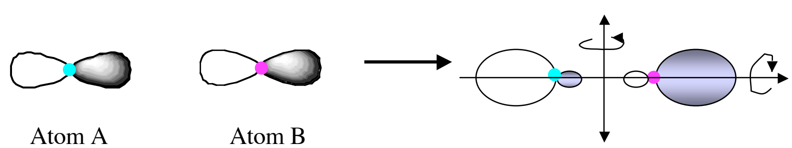
<u>σ*–bond</u> (antibond)

σ since still doesn't change sign upon rotation about internuclear axis



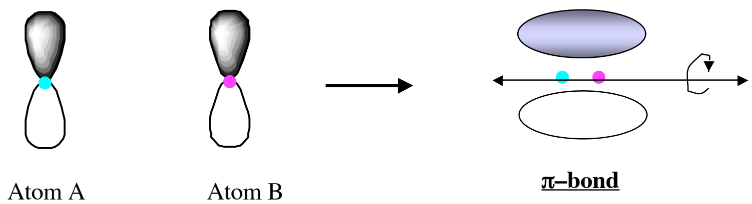
<u>σ–bond</u>

doesn't change sign
upon rotation about
internuclear axis



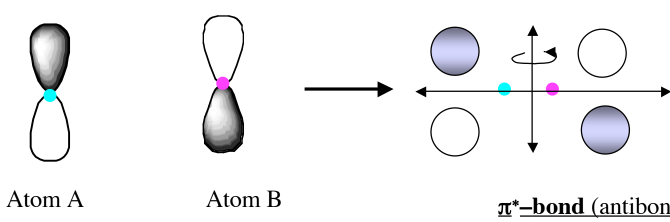
<u>σ*–bond</u> (antibond)

antibonding since changes sign upon rotation about axis perpendicular to internuclear axis



<u>π–bond</u>

changes sign
upon rotation about
internuclear axis

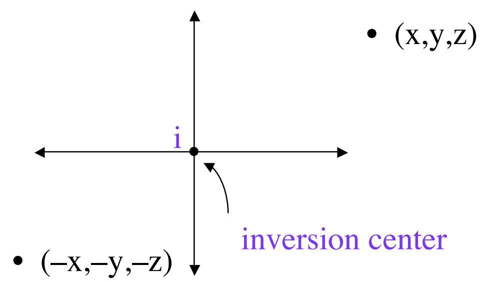


<u>**π*–bond** (antibond)</u>

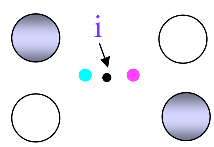
π since still changes sign upon rotation about internuclear axis

antibonding since changes sign upon rotation about axis perpendicular to internuclear axis

Additional orbital labels, used by your book,
describe orbital symmetry with respect to **inversion**

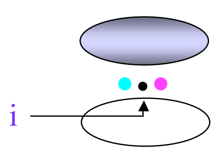


Additional orbital labels, used by your book,
describe orbital symmetry with respect to inversion



π_g^*

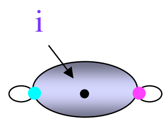
g= gerade, if orbital does <u>not</u>
change phase upon inversion



π_u

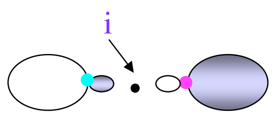
u= ungerade, if orbital <u>does</u>
change phase upon inversion

Additional orbital labels, used by your book, describe orbital symmetry with respect to inversion



σ_g

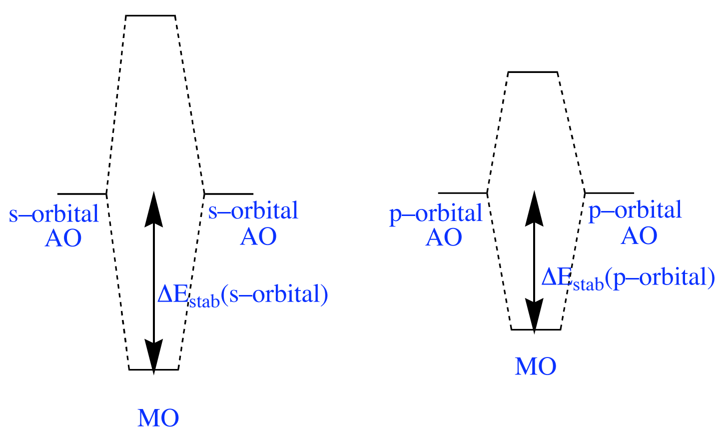
g= gerade, if orbital does <u>not</u> change phase upon inversion



σ_u^*

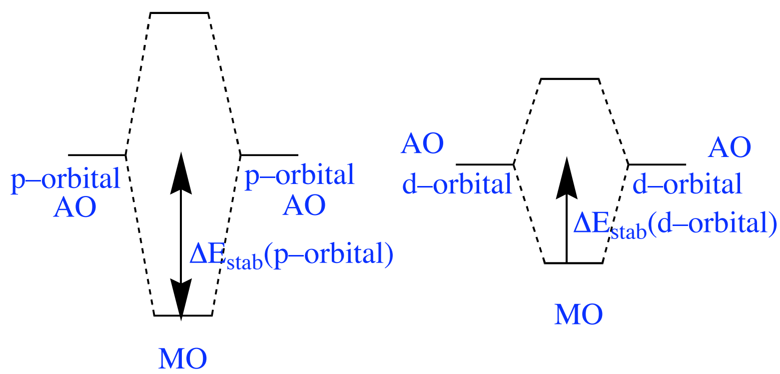
u= ungerade, if orbital <u>does</u> change phase upon inversion

the amount of stabilization and destabilization which results from orbital overlap depends on the type of orbital involved



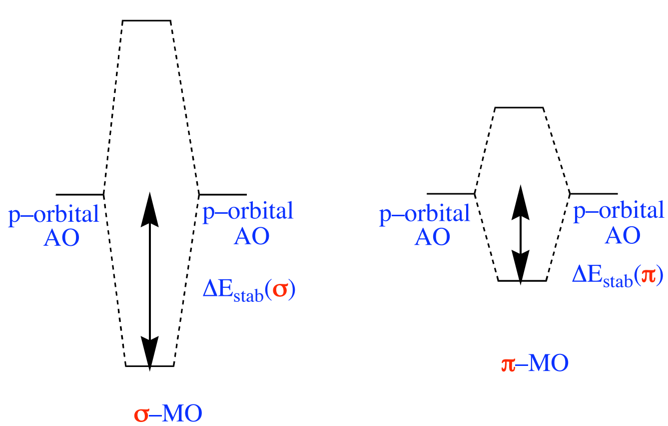
$$\Delta E_{stab}(\text{s-orbital}) >> \Delta E_{stab}(\text{p-orbital})$$

the amount of stabilization and destabilization which results from orbital overlap depends on the type of orbital involved



$$\Delta E_{stab}(\text{p-orbital}) >> \Delta E_{stab}(\text{d-orbital})$$

With <u>p-orbitals</u> need to consider two types of overlap, sigma (σ) and pi (π)



$$\Delta E_{stab}(\text{sigma}) >> \Delta E_{stab}(\text{pi})$$

Sigma overlap is better

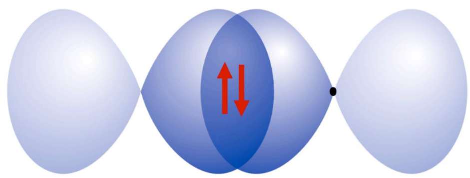


Figure 2-4
Shriver & Atkins Inorganic Chemistry, Fourth Edition

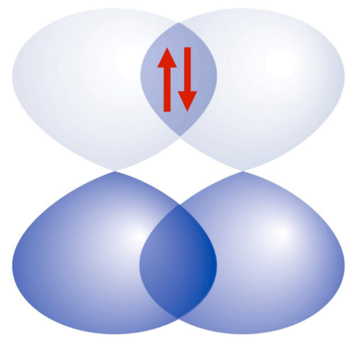
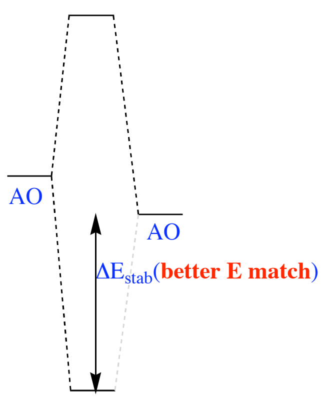


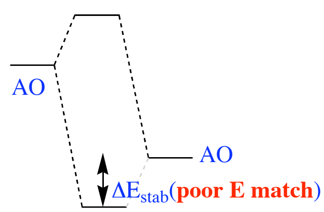
Figure 2-6
Shriver & Atkins Inorganic Chemistry, Fourth Edition

$$\Delta_{stab}(\text{sigma}) >> \Delta_{stab}(\text{pi})$$

One also needs to consider **energy match**



AOs are closer
in energy



AOs are further
apart in energy

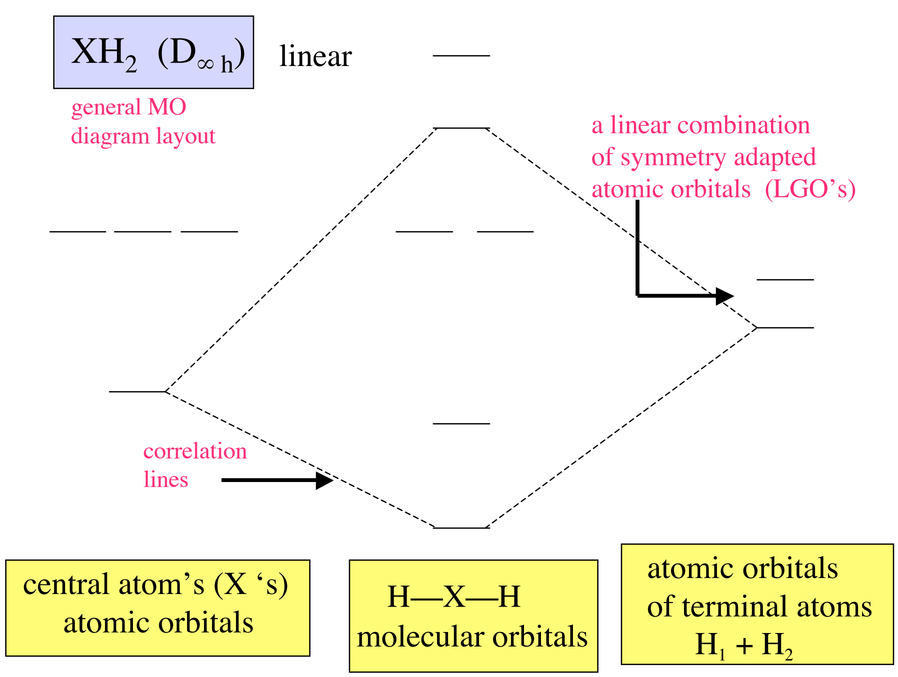
$$\Delta E_{stab}(\text{better E match}) >> \Delta E_{stab}\ (\text{poor E match})$$

Molecular Orbital Diagrams of more complicated molecules

XH_2 ($D_{\infty h}$)

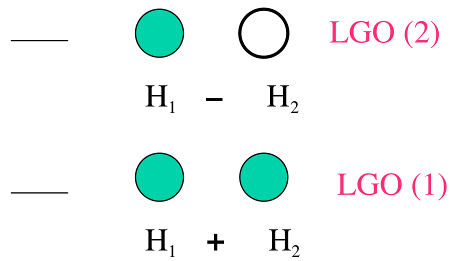
H_2O (C_{2v})

SF_6 (O_h)



a linear combination of symmetry adapted
atomic orbitals (LGO's)…………...

Taken individually, the hydrogen atoms do not possess the symmetry properties of the XH_2 molecule. Taken as a group they do, however.

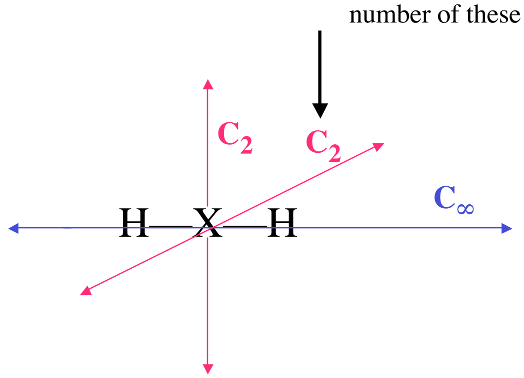


what does this mean………?

atomic orbitals of terminal atoms $H_1 + H_2$

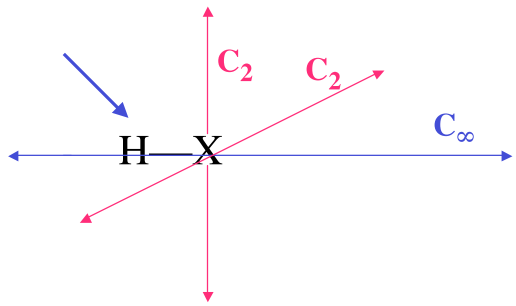
What are the symmetry properties of this molecule?

There are an infinite
number of these



……..and an infinite number
of mirror planes perpendicular
to the C∞ axis, which contain
the C_2's.

Taken individually, this hydrogen atom does not possess C_2 symmetry about axes that are perpendicular to the C_∞.



Thus, the individual hydrogen atoms do not conform to the molecular $D_{\infty h}$ symmetry.

s-orbital symmetry label

XH_2's point group

symmetry label given to identify the p_z orbital of atom X (central atom)

atom X's p_z atomic orbitals

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

symmetry label given to identify the p_x and p_y orbitals of atom X (central atom)

atom X's p_x and p_y atomic orbitals

atom X's s–orbital

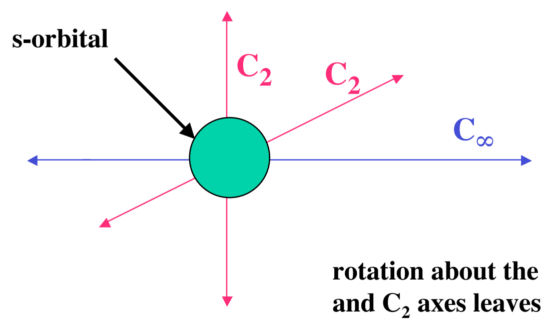
- We can perform symmetry operations on orbitals as well as molecules

- We can perform symmetry operations on orbitals as well as molecules

- the rows of numbers that follow each orbitals symmetry label tell us how that orbital behaves when operated upon by each symmetry element

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

- We can perform symmetry operations on orbitals as well as molecules
- the rows of numbers that follow each orbitals symmetry label tell us how that orbital behaves when operated upon by each symmetry element
- a "1" means that the orbital is unchanged by the symmetry operation
- a "**–1**" means that the orbital changes phase as a result of the symmetry operation
- a "0" means that the orbital changes in some other way as a result of the symmetry operation
- a "**cos θ**" occurs with degenerate sets of orbitals (eg. (p_x, p_x)) that take on partial character of one another upon performance of a symmetry operation



rotation about the C_∞, and C_2 axes leaves the s–orbital unchanged

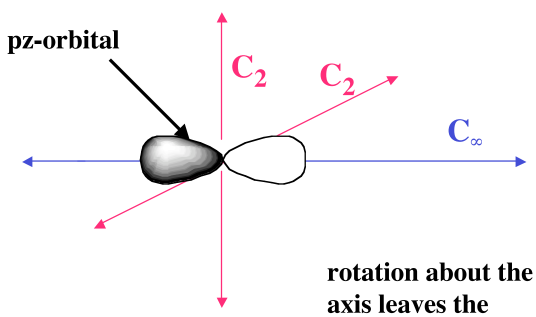
thus the “1” <u>character</u> in the row highlighted for the s-orbital, and under the columns headed C_∞, and ∞C_2

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

on the other hand, the p_z orbital changes phase upon rotation about any of the C_2 axes

$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_{\phi}$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, $x^2 + y^2$
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		$(xy, x^2 - y^2)$
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

rotation about the C_2 axis changes the phase of the pz orbital pz–orbital



rotation about the C_∞ axis leaves the pz–orbital unchanged

…but a +1 "plus one" under the column headed C_∞

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

thus the "–1" (negative one) <u>character</u>
in the column headed C_2

When the px and py are rotated about the C_∞ axis,
they move, rather than transform into themselves

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

Thus the "0" in the column labeled $2C_\infty$

inversion, on the other hand, causes both the px and py to change phase

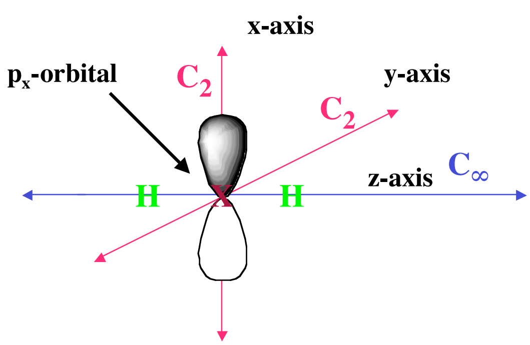
$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
$A_{1g}\ (\Sigma_g^+)$	1	1	1	1	1	1		$z^2,\ x^2+y^2$
$A_{1u}\ (\Sigma_u^+)$	1	1	−1	−1	1	−1	z	
$A_{2g}\ (\Sigma_g^-)$	1	−1	1	1	−1	1	R_z	
$A_{2u}\ (\Sigma_u^-)$	1	1	1	−1	−1	−1		
$E_{1g}\ (\Pi_g)$	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	$(R_x,\ R_y)$	$(zx,\ yz)$
$E_{1u}\ (\Pi_u)$	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	$(x,\ y)$	
$E_{2g}\ (\Delta_g)$	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		$(xy,\ x^2-y^2)$
$E_{2u}\ (\Delta_u)$	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

Thus the "–2" in the column labeled *i*

The "–2" indicates that <u>both</u> orbitals transform as <u>a set</u>

the orbitals are defined in terms of a fixed coordinate system

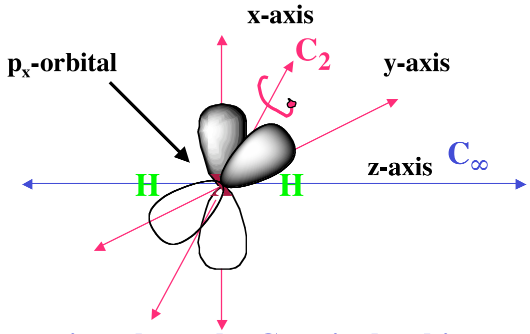
Rotation about the C_∞ axis moves thep_x–orbital into a position where it no longer looks like a px orbital



The z-axis is selected so that it either coincides with the highest-fold rotation axis, or the internuclear axis, or both

For all C_2's except those that coincide with the x- and y-axes, rotation about C_2 causes the p_x–orbital to take on some p_y –orbital character

Rotation about the $C_{2's}$ that do not coincide with the x- or y-axes, causes the p_x–orbital to take on some p_y –orbital character



In fact, rotation about the C_2 axis that bisects the x- and y-axes converts the p_x–orbital into the p_y –orbital. **This indicates that these two orbitals must be degenerate (ie have identical energies)**

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

Thus the "cos φ" term in the column labeled ∞C_2

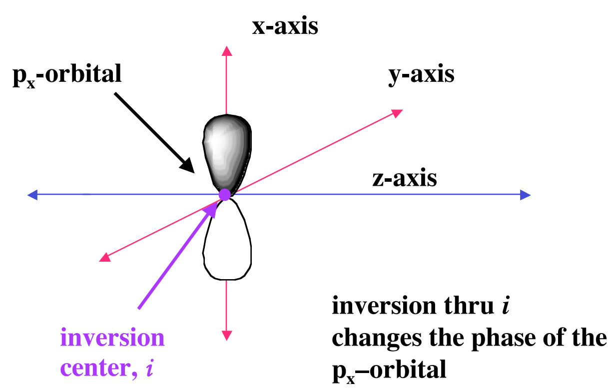
The number in the "E" column tells you how many orbitals transform together as a set

inversion, on the other hand, causes both the px and py to change phase, but maintain their identities

$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

Thus the "–2" in the column labeled *i*

The "–2" indicates that <u>both</u> orbitals transform as <u>a set</u>



Thus, we have determined the symmetry labels, generally referred to as Mulliken symbols, for the s and p_z, p_x,and p_y-orbitals on the central atom X

XH_2 ($D_{\infty h}$)

This explains the labels shown for the central atom X on the left

p_z p_x p_y

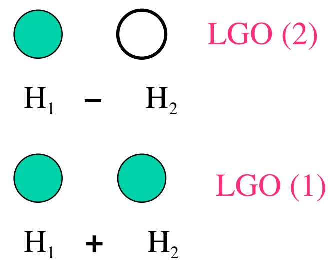
$\mathbf{a_{1u}}$ (σ_u) $\mathbf{e_{1u}}$ (π_u)

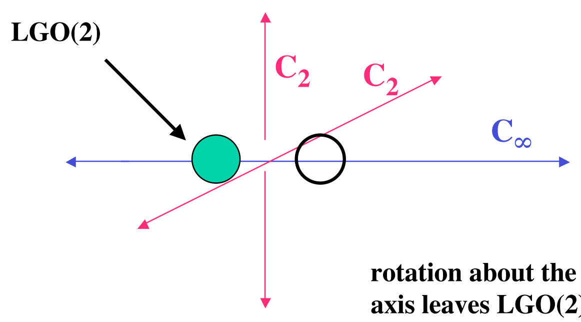
2s

$\mathbf{a_{1g}}$ (σ_g)

central atom's (X 's) atomic orbitals

We determine the symmetry labels for the LGO's in the same manner, ie., by examining their symmetry with respect to the symmetry operations of the $D_{\infty h}$ point group

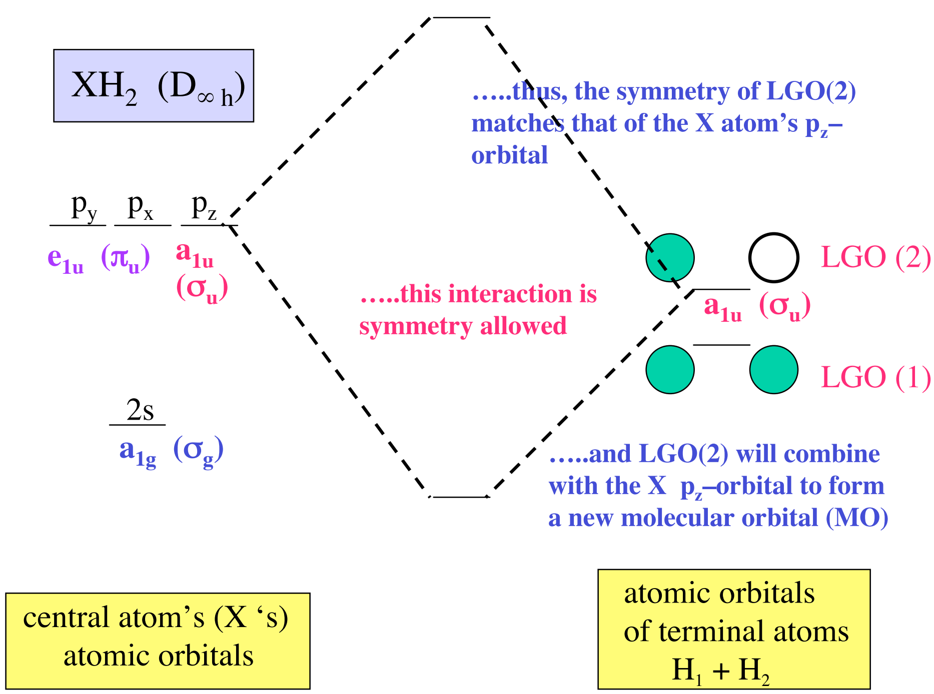




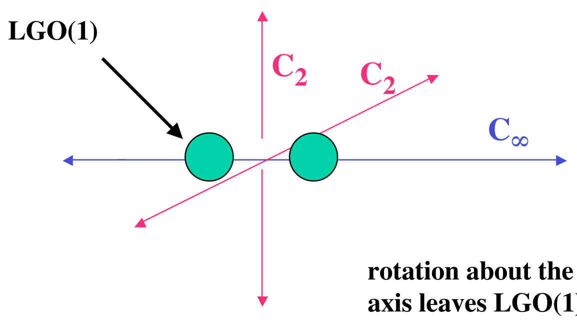
……thus it appears that LGO(2) possesses a_{1u} symmetry

$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_{\phi}$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, x^2+y^2
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

…… symmetry identical to that of the central atom X's p_z orbital



rotation about the C_2 axes leaves LGO(1) unchanged



rotation about the C_∞ axis leaves LGO(1) unchanged

Or….

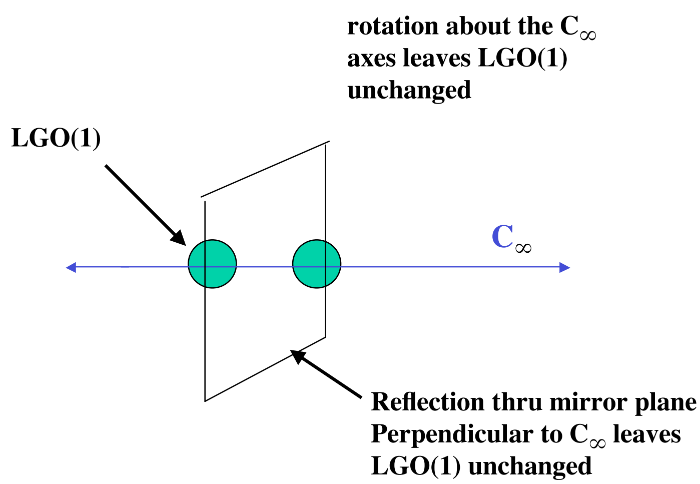
…...thus it appears that LGO(1) could possess either a_{1g} , or a_{2u} symmetry

$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	$\boxed{1}$	$\boxed{1}$	1	1	1		$\boxed{z^2, x^2+y^2}$
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	$\boxed{1}$	$\boxed{1}$	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, x^2-y^2)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

…... a_{1g} would match orbitals on atom X, whereas a_{2u} would not.

……if we examine the symmetry of LGO(1) with respect to both inversion, and reflection, we should be able to distinguish between these two options

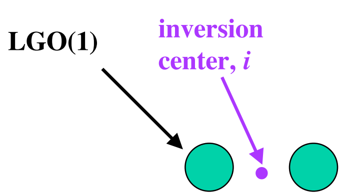
$D_{\infty h}$	E	$2C'_\infty$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
A_{1g} (Σ_g^+)	1	1	1	1	1	1		z^2, $x^2 + y^2$
A_{1u} (Σ_u^+)	1	1	−1	−1	1	−1	z	
A_{2g} (Σ_g^-)	1	−1	1	1	−1	1	R_z	
A_{2u} (Σ_u^-)	1	1	1	−1	−1	−1		
E_{1g} (Π_g)	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	(R_x, R_y)	(zx, yz)
E_{1u} (Π_u)	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	(x, y)	
E_{2g} (Δ_g)	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		(xy, $x^2 - y^2$)
E_{2u} (Δ_u)	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		



……thus, we can rule out a_{2u} as the symmetry assignment for LGO(1), based on reflection, and improper rotation

$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_{\phi}$	$h = \infty$	
$\boxed{A_{1g}\ (\Sigma_g^+)}$	1	1	1	$\boxed{1}$	$\boxed{1}$	$\boxed{1}$		$z^2,\ x^2 + y^2$
$A_{1u}\ (\Sigma_u^+)$	1	1	−1	−1	1	−1	z	
$A_{2g}\ (\Sigma_g^-)$	1	−1	1	1	−1	1	R_z	
$\boxed{\cancel{A_{2u}\ (\Sigma_u^-)}}$	1	1	1	$\boxed{-1}$	$\boxed{\cancel{-1}}$	$\boxed{\cancel{-1}}$		
$E_{1g}\ (\Pi_g)$	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	$(R_x,\ R_y)$	$(zx,\ yz)$
$E_{1u}\ (\Pi_u)$	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	$(x,\ y)$	
$E_{2g}\ (\Delta_g)$	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		$(xy,\ x^2 - y^2)$
$E_{2u}\ (\Delta_u)$	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

inversion leaves LGO(1) unchanged



……thus, we can rule out a_{1u}, and a_{2u} as the symmetry assignment for LGO(1)

$D_{\infty h}$	E	$2C'_{\infty}$	∞C_2	i	$\infty\sigma_v$	$2S_\phi$	$h = \infty$	
$\boxed{A_{1g}\ (\Sigma_g^+)}$	1	1	1	$\boxed{1}$	1	1		$z^2,\ x^2+y^2$
$A_{1u}\ (\Sigma_u^+)$	1	1	−1	$\cancel{-1}$	1	−1	z	
$A_{2g}\ (\Sigma_g^-)$	1	−1	1	1	−1	1	R_z	
$A_{2u}\ (\Sigma_u^-)$	1	1	1	$\cancel{-1}$	−1	−1		
$E_{1g}\ (\Pi_g)$	2	0	$2\cos\phi$	2	0	$-2\cos\phi$	$(R_x,\ R_y)$	$(zx,\ yz)$
$E_{1u}\ (\Pi_u)$	2	0	$2\cos\phi$	−2	0	$2\cos\phi$	$(x,\ y)$	
$E_{2g}\ (\Delta_g)$	2	0	$2\cos 2\phi$	2	0	$2\cos 2\phi$		$(xy,\ x^2-y^2)$
$E_{2u}\ (\Delta_u)$	2	0	$2\cos 2\phi$	−2	0	$-2\cos 2\phi$		
⋮	⋮	⋮	⋮	⋮	⋮	⋮		

……leaving a_{1g} as the symmetry assignment for LGO(1)

XH_2 ($D_{\infty h}$)

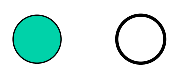
…..thus, the symmetry of LGO(1) matches that of the X atom's s–orbital

p_z p_x p_y

a_{1u} (σ_u) e_{1u} (π_u)

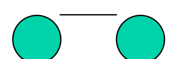
2s

a_{1g} (σ_g)



LGO (2)

a_{1u} (σ_u)



LGO (1)

a_{1g} (σ_g)

central atom's (X 's) atomic orbitals

atomic orbitals of terminal atoms $H_1 + H_2$

…..inserting our correlation lines between orbitals of the same symmetry