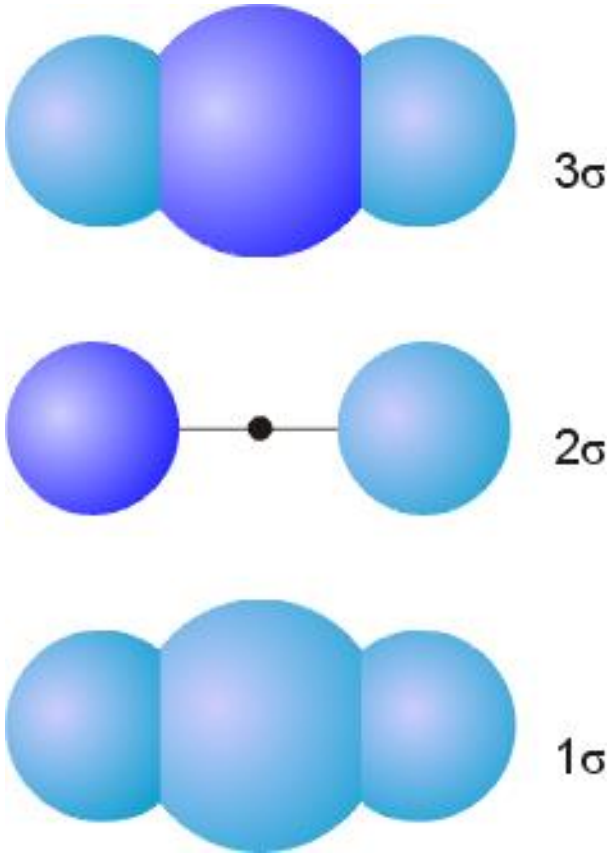
MO Theory of Polyatomic Systems

$H_3^{+/\cdot/-}$ Two extreme cases: linear or cyclic

- Increasing number of nodal planes



MO Theory of Polyatomic Systems

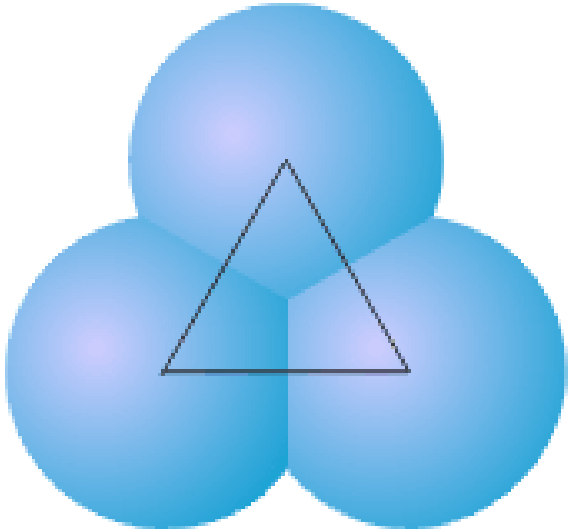
$H_3^{+/\cdot/-}$ cyclic

D_{3h} ($\bar{6}m2$)	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	$h = 12$	
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(zx, yz)

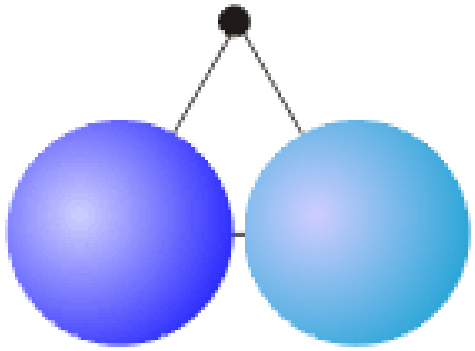
MO Theory of Polyatomic Systems

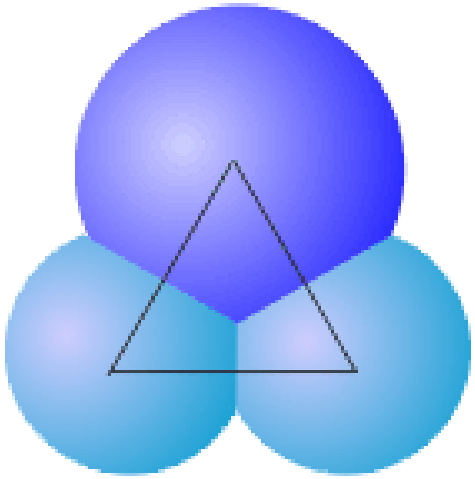
$H_3^{+/\cdot/-}$

D_{3h} ($\bar{6}m2$)	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	$h = 12$	
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(zx, yz)



a_1

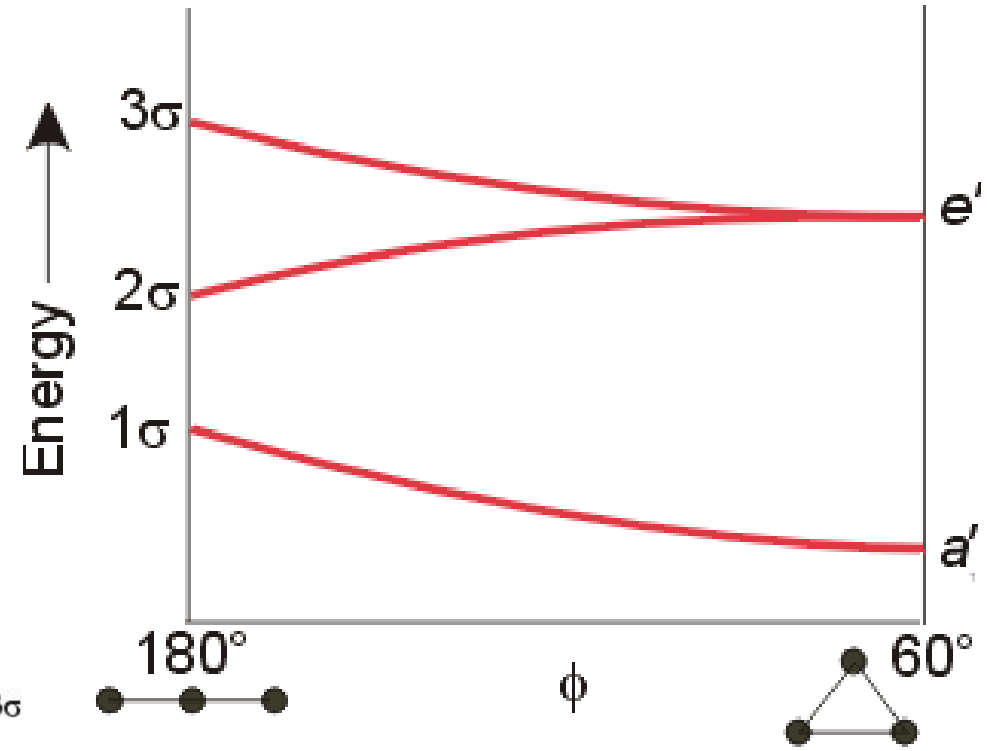


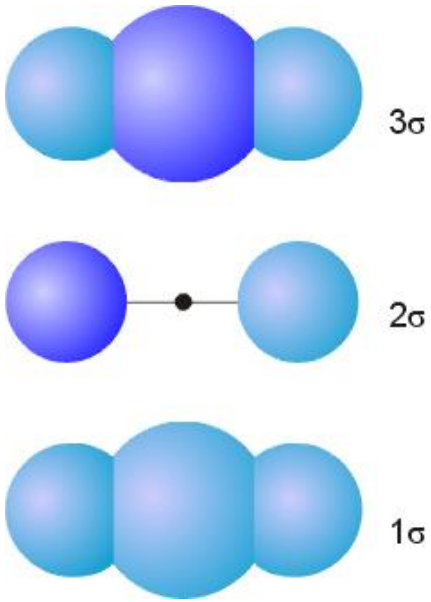


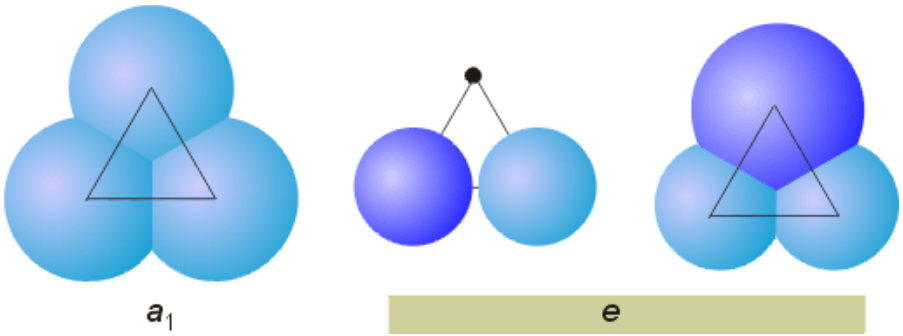
e

Walsh Diagram of H_3

$H_3^{+/\cdot/-}$







MO Theory of Polyatomics: The Central-Atom Model

- Determine the point group of the molecule.

- Consider the atomic orbitals from the central atom:
  - get symmetry labels for those AOs

- Consider atomic orbitals from the peripheral atoms (ligand atoms):
  - get sets of symmetry adapted orbitals.

- Combine AOs to MOs according to rules of symmetry, energy and overlap