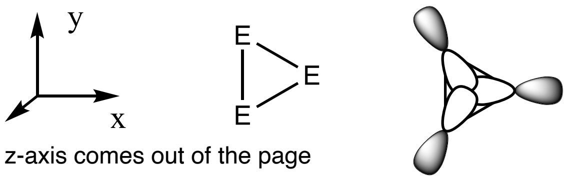
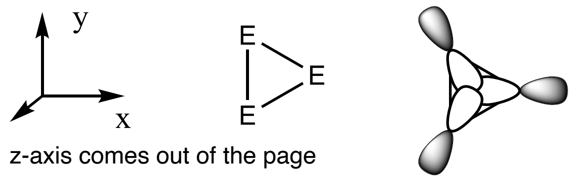
- A fragment E_3 belongs to the D_{3h} point group and consists of three atoms (E) arranged in an equilateral triangle as shown below. Determine the symmetry adapted FOs for the 3 in-plane pAOs **A** of this fragment.



- A fragment E_3 belongs to the D_{3h} point group and consists of three atoms (E) arranged in an equilateral triangle as shown below. Determine the symmetry adapted FOs for the 3 in-plane pAOs **A** of this fragment.



- D_{3h} character table

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	σ_v		
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	(T_x, T_y)	x^2-y^2, xy
A_1”	1	1	1	−1	−1	−1		
A_2”	1	1	−1	−1	−1	1	T_z	
E”	2	−1	0	−2	1	0	(R_x, R_y)	xz, yz

- First find the reducible representation (**Γ_A**) for the basis set **A**
  - determined by the orbitals that do not move under each operation

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
Γ_A	3	0	1	3	0	1

- Determine the contributing irreducible representations
  - using appropriate short cuts
  - always show your working
  - The first IR will likely be the totally symmetric A_1' so try this first
  - then subtract from the reducible representation, and identify this belongs to E'

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
Γ_A	3	0	1	3	0	1
A_1'	1	1	1	1	1	1

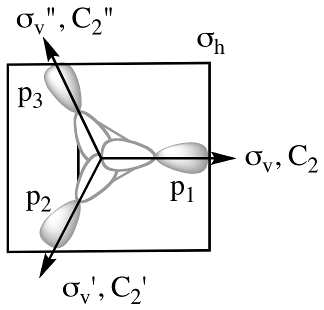
$$n_{A'_1} = \frac{1}{12}\left[(1\cdot 3\cdot 1)+(2\cdot 0\cdot 1)+(3\cdot 1\cdot 1)+(1\cdot 3\cdot 1)+(2\cdot 0\cdot 1)+(3\cdot 1\cdot 1)\right]$$

$$= \frac{1}{12}\left[3+0+3+3+0+3\right] = \frac{12}{12} = 1$$

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	
Γ_D	3	0	1	3	0	1	
A_1'	1	1	1	1	1	1	
$\Gamma_A - A_1'$	2	-1	0	2	-1	0	=E'

- Use the projection formula to determine the wavefunctions
  - shown here is one wavefunction for the degenerate irreducible representation.
  - draw the molecular orbital.

		$2C_3$		$3C_2$				$2S_3$		3σ		
D_{3h}	E	C_3^1	C_3^2	C_2	C_2'	C_2''	σ_h	S_3^1	S_3^2	σ	σ'	σ''
$Q[p_1]$	p_1	p_2	p_3	p_1	p_3	p_2	p_1	p_2	p_3	p_1	p_3	p_2
E'	2	-1	-1	0	0	0	2	-1	-1	0	0	0
$\chi^{E''}(Q)\bullet Q\bullet[p_1]$	$2p_1$	$-p_2$	$-p_3$	0	0	0	$2p_1$	$-p_2$	$-p_3$	0	0	0

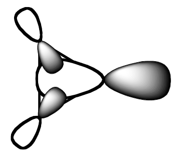


C3 axis comes out of the page
S3 axis coincident with C3 axis

$$P_{E'}[p_1] = \frac{1}{12}[2p_1 - p_2 - p_3 + 0 + 2p_1 - p_2 - p_3 + 0]$$

$$\psi_{E'} = P_{E'}[p_1] = \frac{1}{12}[4p_1 - 2p_2 - 2p_3] = \frac{1}{6}[2p_1 - p_2 - p_3]$$

$$\psi_{e'}(1) = \frac{1}{6}[2p_1 - p_2 - p_3]$$



  - This is a picture of a the real MO of O_3