Character Tables

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Outline

What Makes Up a Character Table

Character tables contain information about how functions transform in response to the operations of the group

Five parts of a character table

1. At the upper left is the symbol for the point group
2. The top row shows the operations of the point group, organized into classes
3. The left column gives the Mulliken symbols for each of the irreducible representations
4. The rows at the center of the table give the characters of the irreducible representations
5. Listed at right are certain functions, showing the irreducible representation for which the function can serve as a basis

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The C_{2v} Character Table

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

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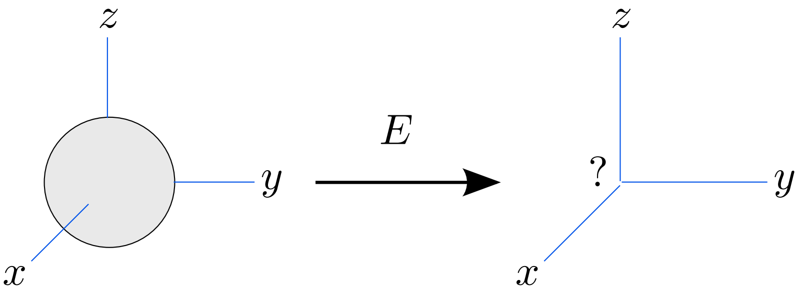
Transformation Properties of an s Orbital in C_{2v}

What happens when the E operation is applied?



- The E operation is a rotation by 360° about an arbitrary axis

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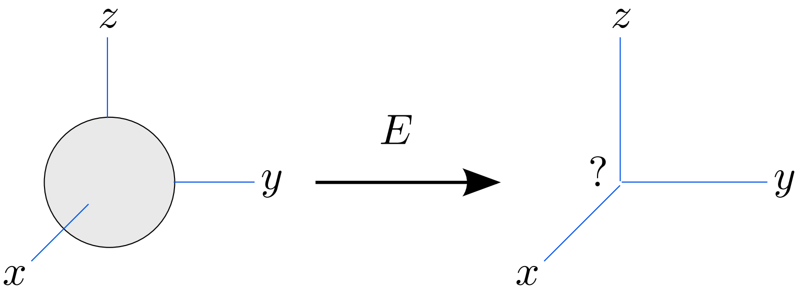

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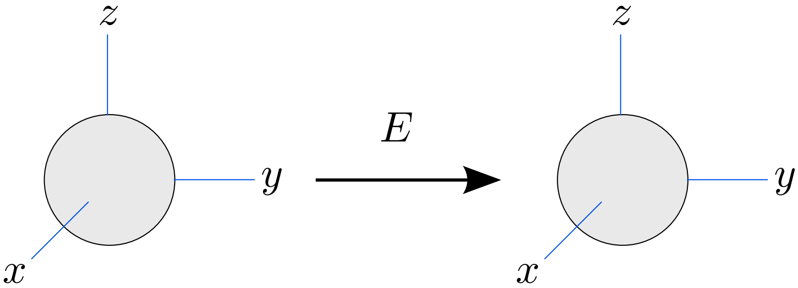

- The result of this corresponds to a character of 1

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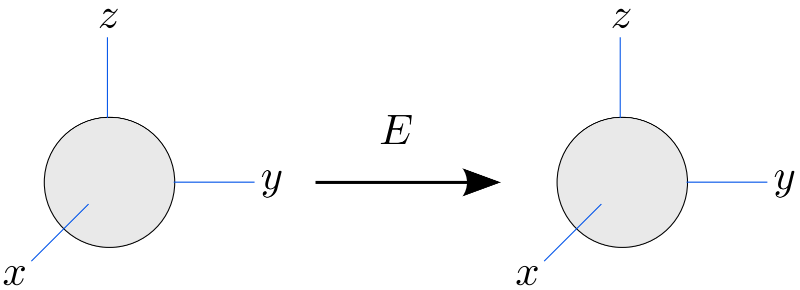

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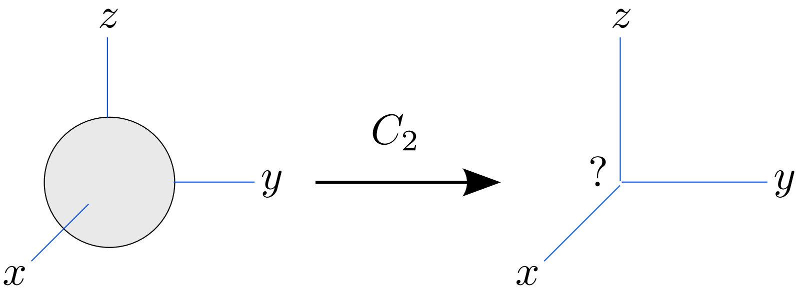

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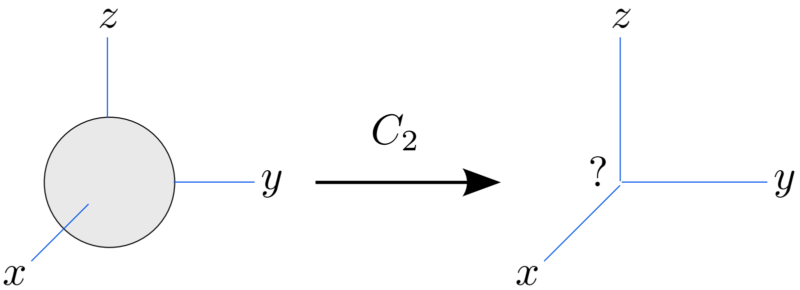

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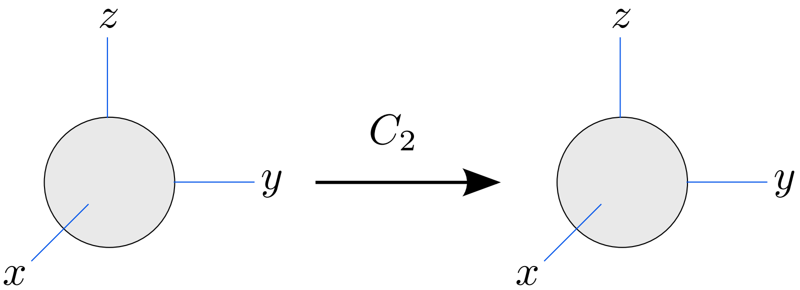

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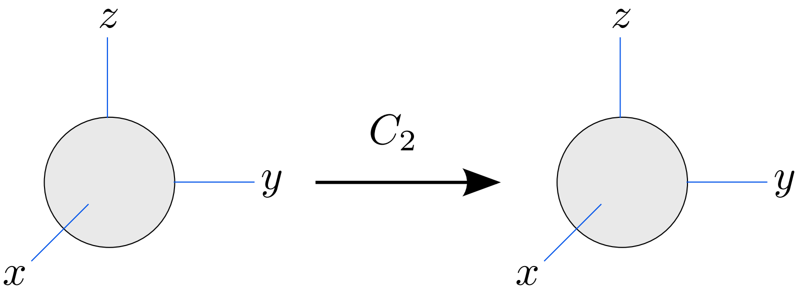

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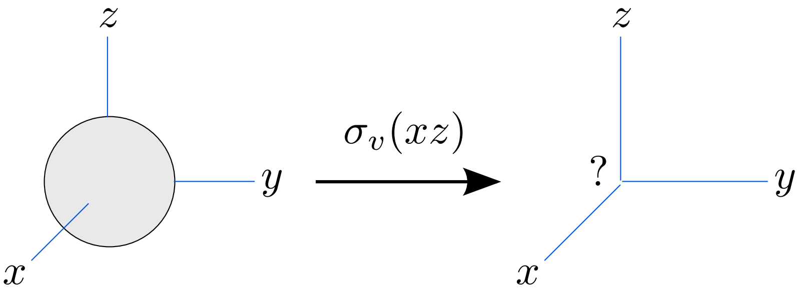

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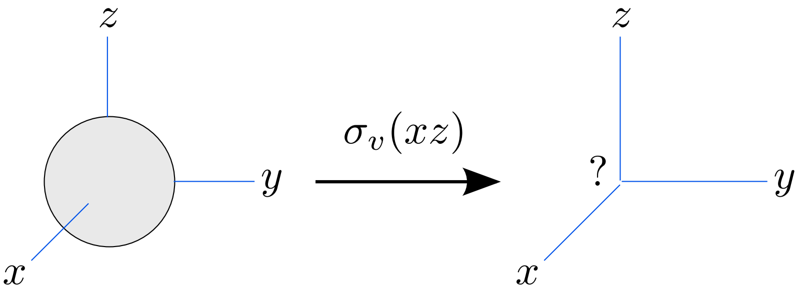

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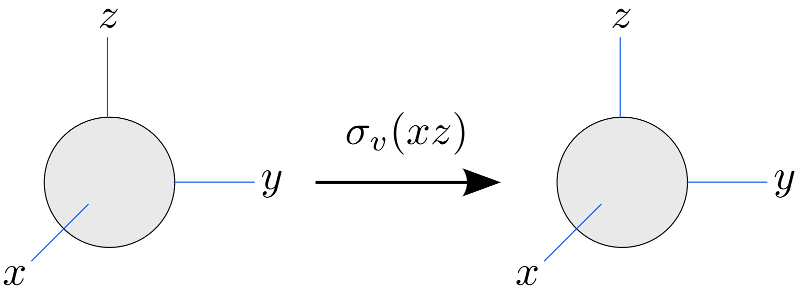

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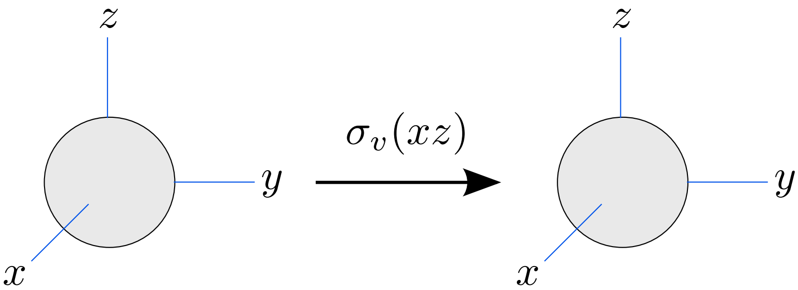

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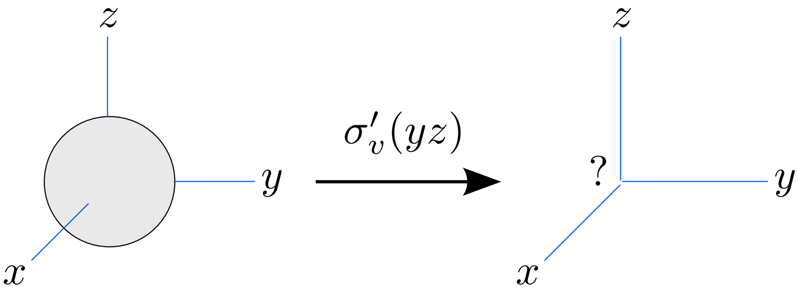

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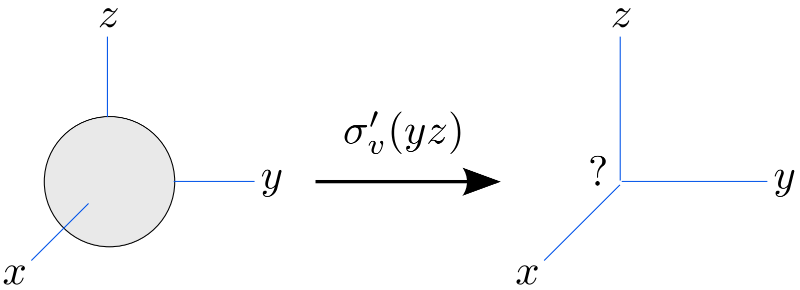

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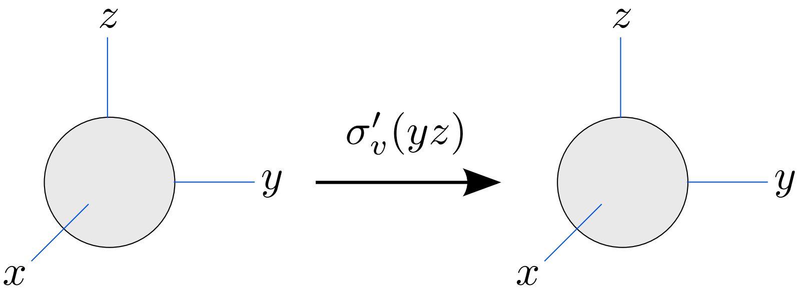

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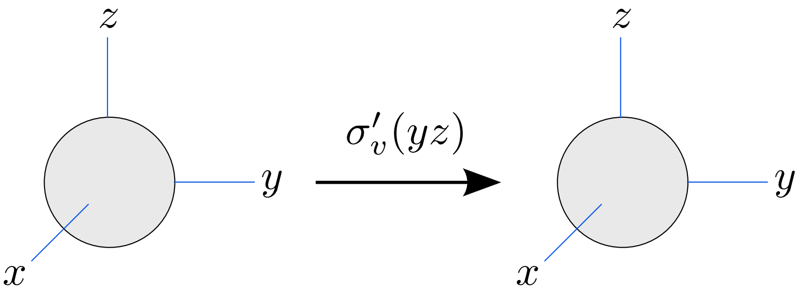

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Transformation Properties of an *s* Orbital

These observations pertain to any central-atom *s* orbital in any point group

- Consider an *s* orbital located on a central atom
- An example of a central atom is O in the case of water, or N in the case of ammonia
- Carrying out any operation on a central atom *s* orbital returns the *s* orbital in its original configuration
- The central-atom *s* orbital "belongs to" or "serves as a basis for" the totally symmetric (A_1) irreducible representation
- All the characters of the totally symmetric irreducible representation are 1
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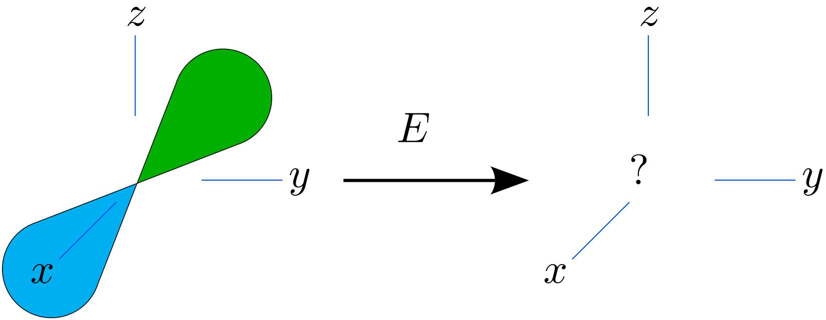

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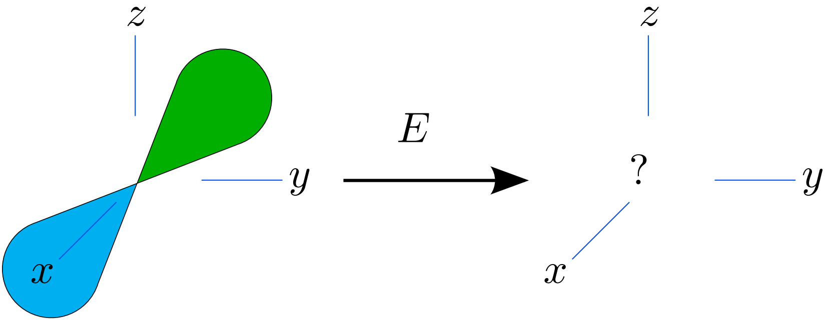

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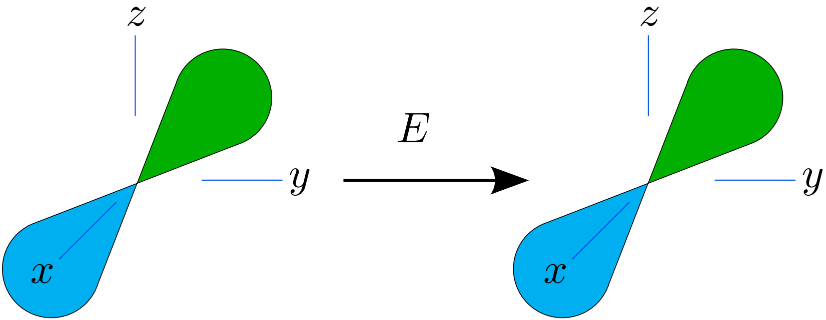

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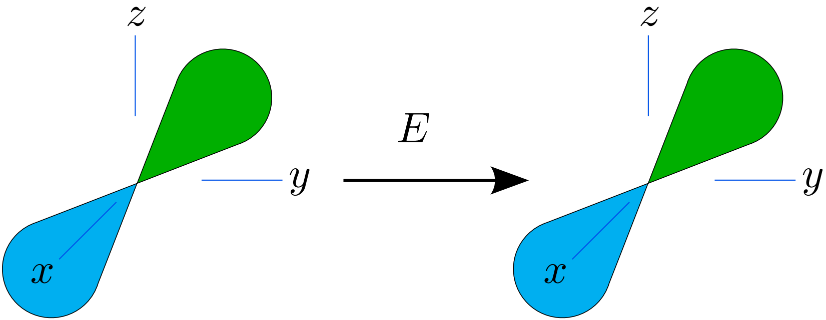

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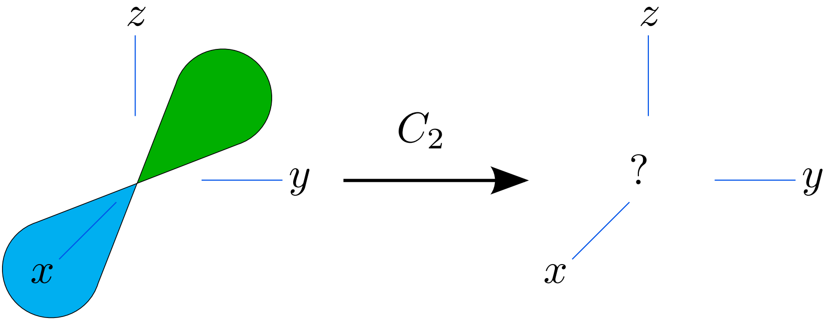

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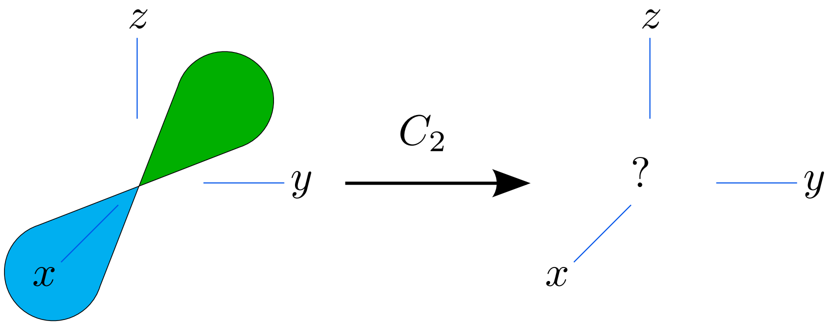

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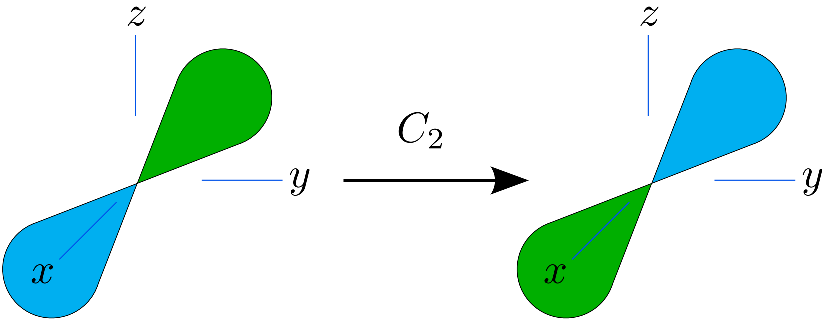
Transformation Properties of a p_x Orbital in C_{2v}

The C_2 operation inverts the phase of the p_x orbital



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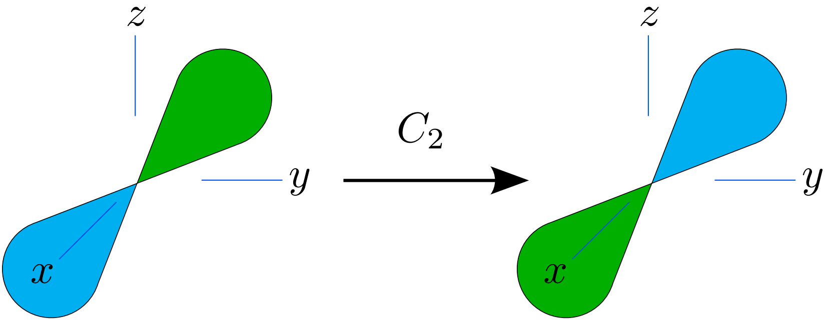

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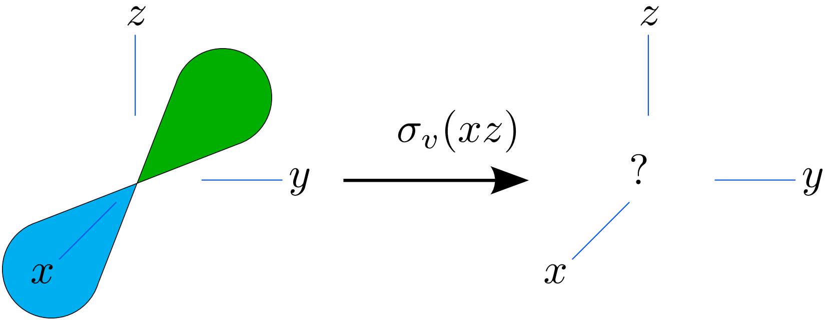

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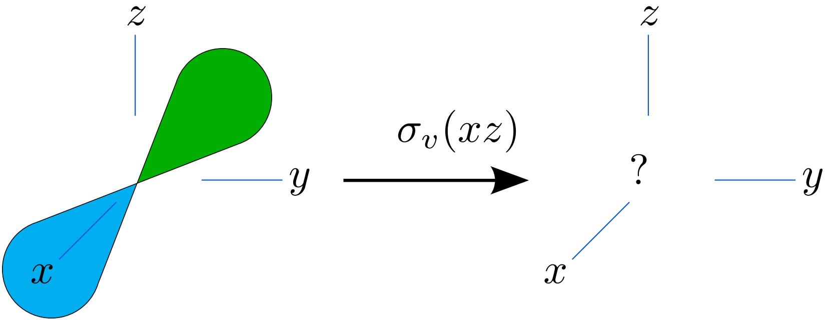

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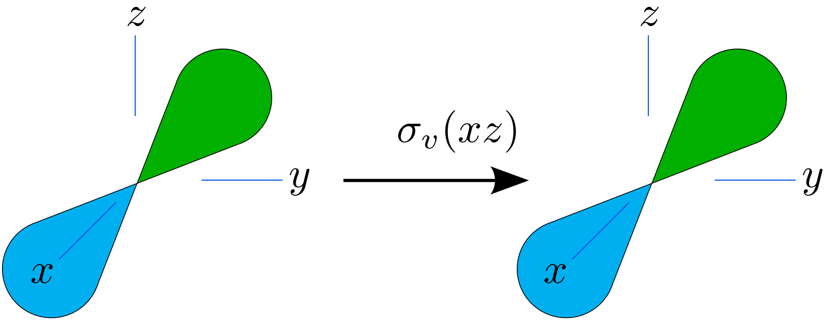
The $\sigma_v(xz)$ operation does nothing to the phase of the p_x orbital



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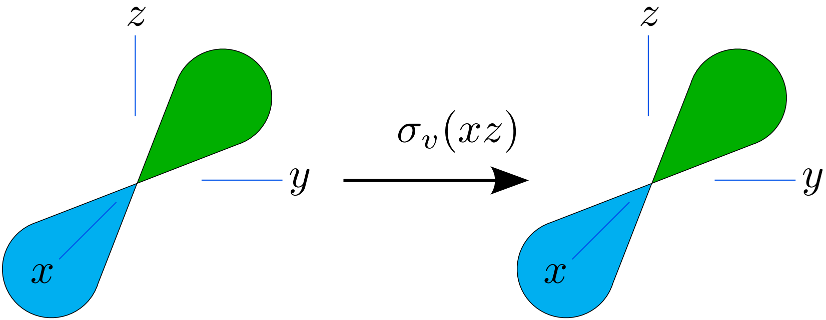

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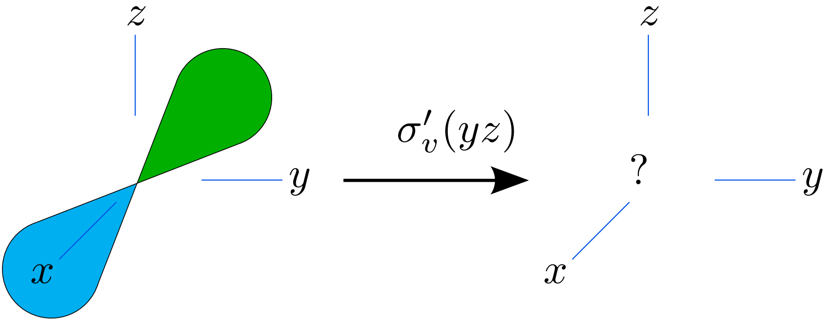

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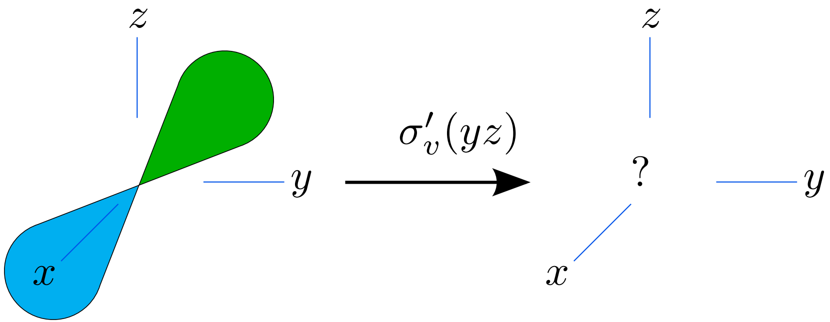

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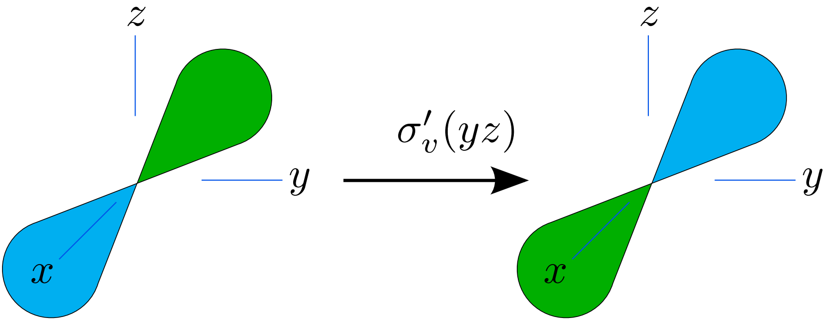

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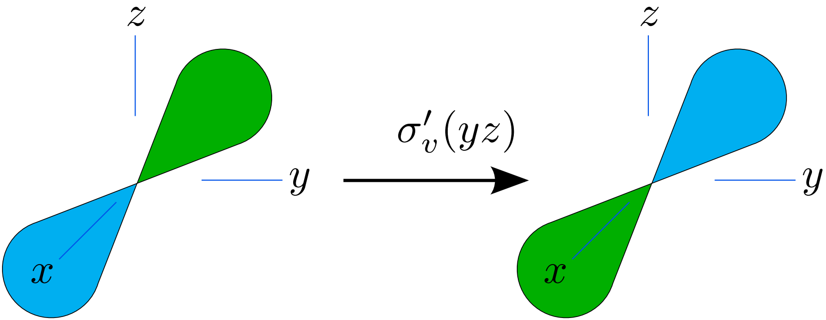

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A p_x Orbital has B_1 Symmetry in C_{2v}

- We carried out the operations of C_{2v} on a central-atom p_x orbital
- This generated the following row of characters: $1, -1, 1, -1$
- This row of characters in the C_{2v} character table is labeled B_1
- Any orbital having these transformation properties in C_{2v} is said to have B_1 symmetry

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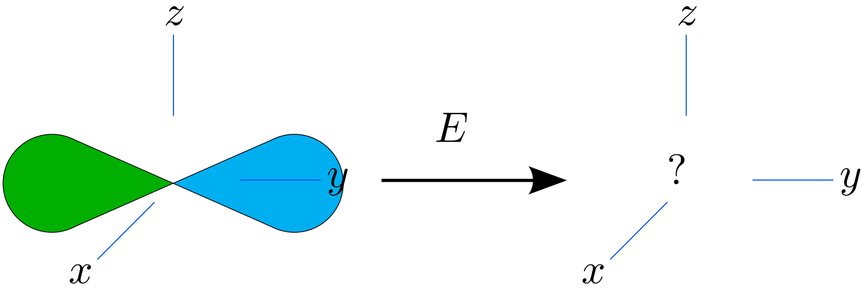

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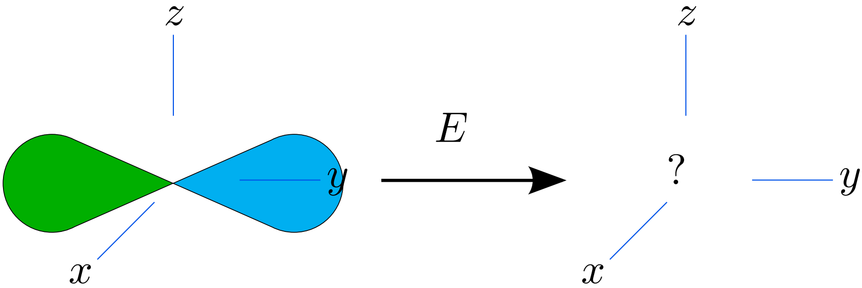

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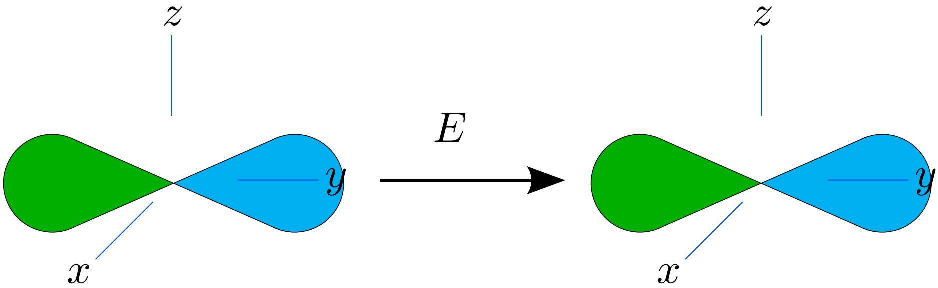
Transformation Properties of a p_y Orbital in C_{2v}

The E operation returns the original configuration of the p_y orbital



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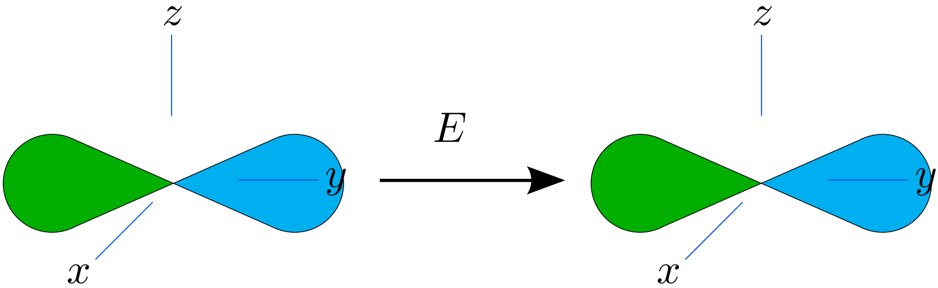

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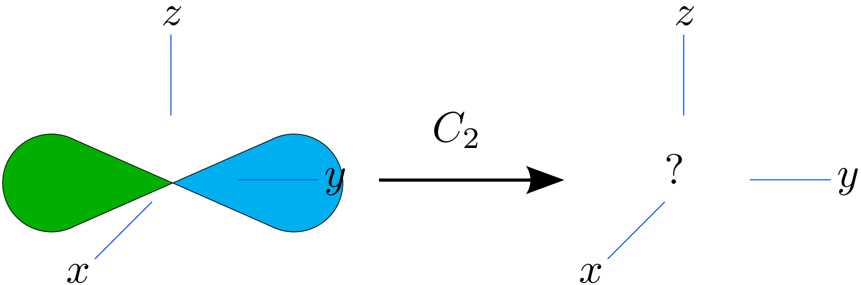

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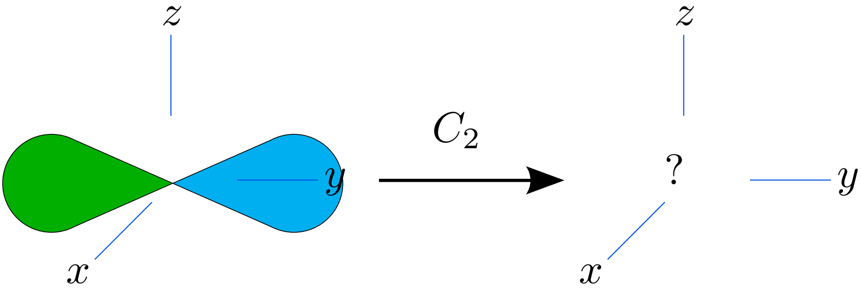

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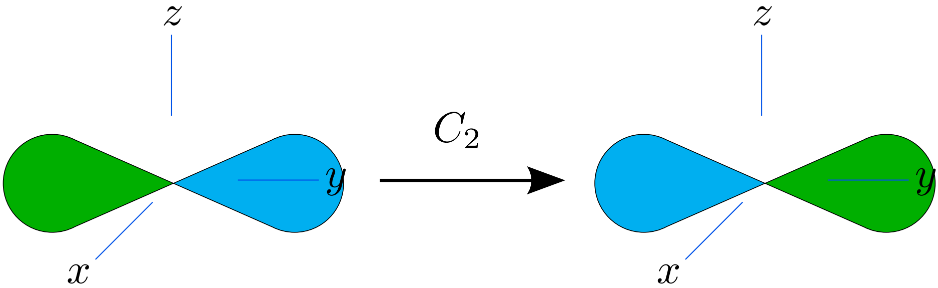
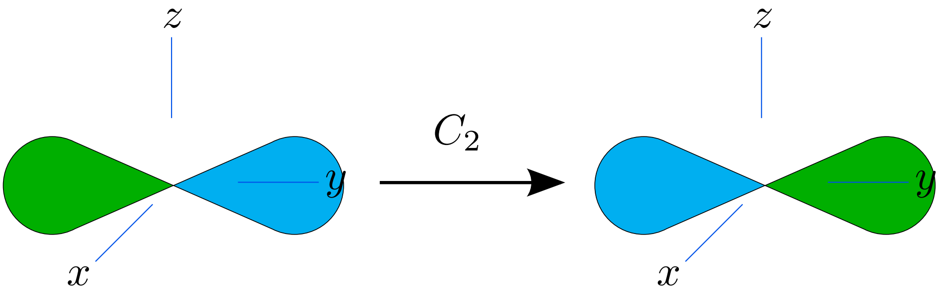
The C_2 operation inverts the phase of the p_y orbital



- The result of this corresponds to a character of -1

Transformation Properties of a p_y Orbital in C_{2v}

The C_2 operation inverts the phase of the p_y orbital



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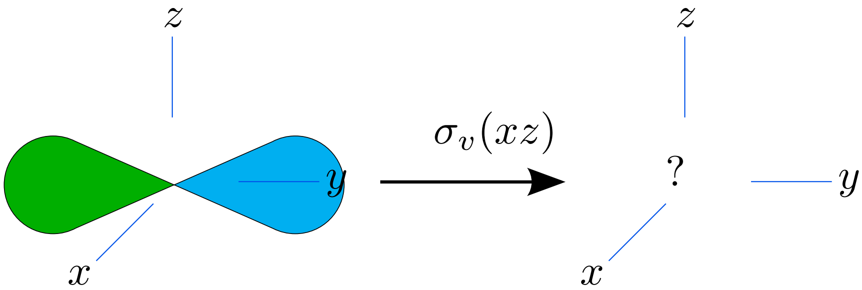
Transformation Properties of a p_y Orbital in C_{2v}

What happens when the $\sigma_v(xz)$ operation is applied?



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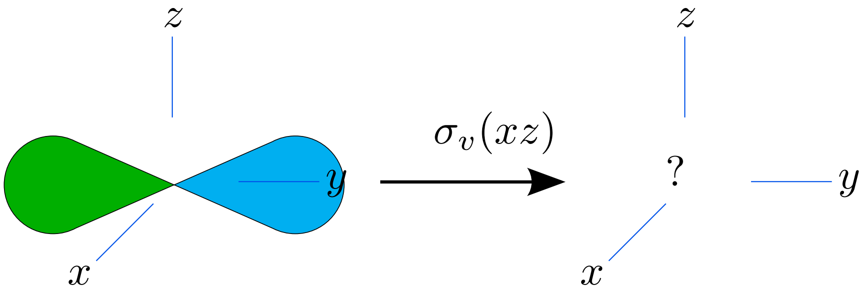

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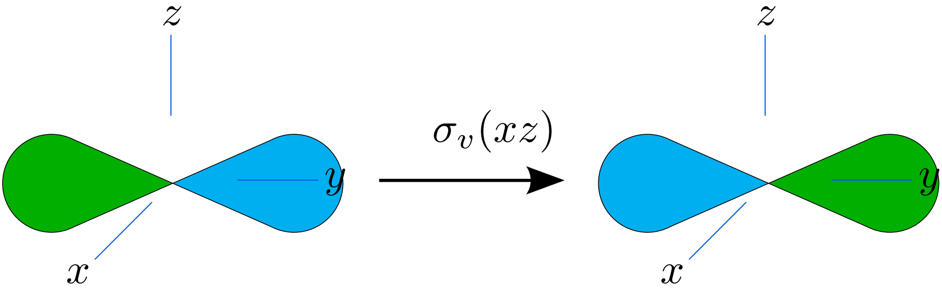

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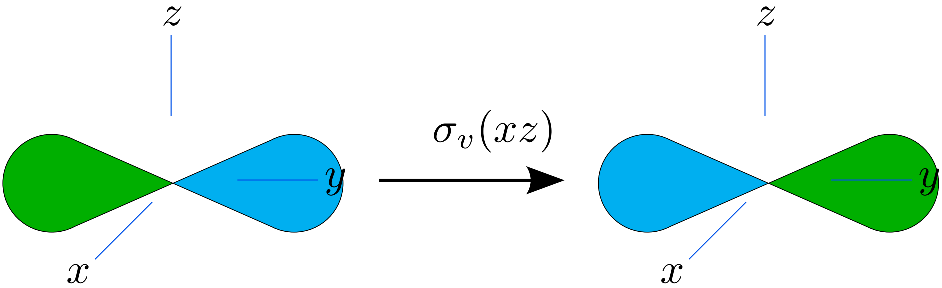

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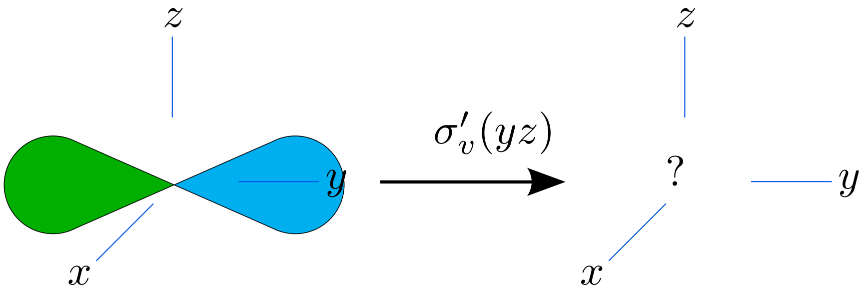

- The $\sigma_v'(yz)$ operation is a reflection through the yz plane

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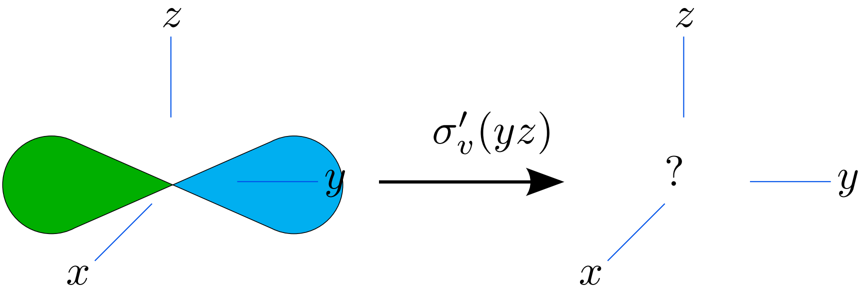

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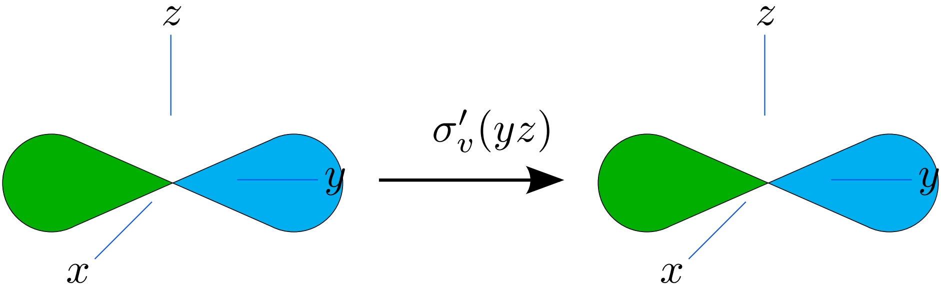
Transformation Properties of a p_y Orbital in C_{2v}

The $\sigma_v'(yz)$ operation does nothing to the phase of the p_y orbital



- The result of this corresponds to a character of 1

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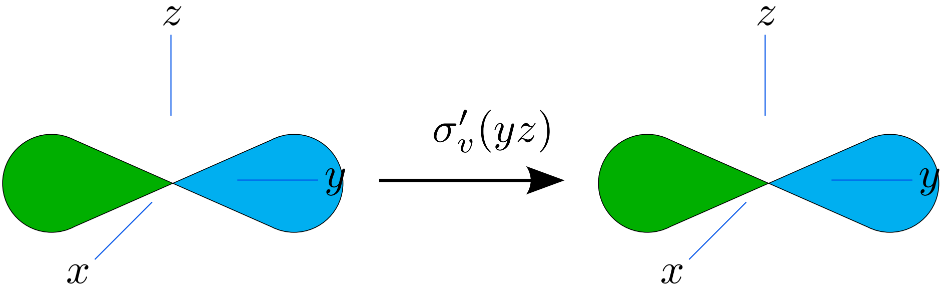

- The result of this corresponds to a character of 1

A p_y Orbital has B_2 Symmetry in C_{2v}

- We carried out the operations of C_{2v} on a central-atom p_y orbital
- This generated the following row of characters: $1, -1, -1, 1$
- This row of characters in the C_{2v} character table is labeled B_2
- Any orbital having these transformation properties in C_{2v} is said to have B_2 symmetry

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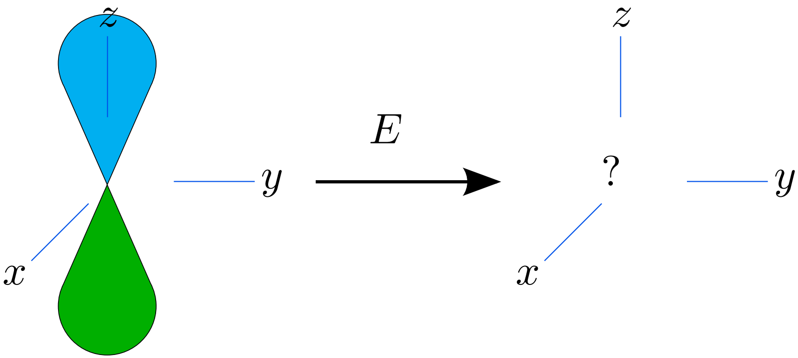
Transformation Properties of a p_z Orbital in C_{2v}

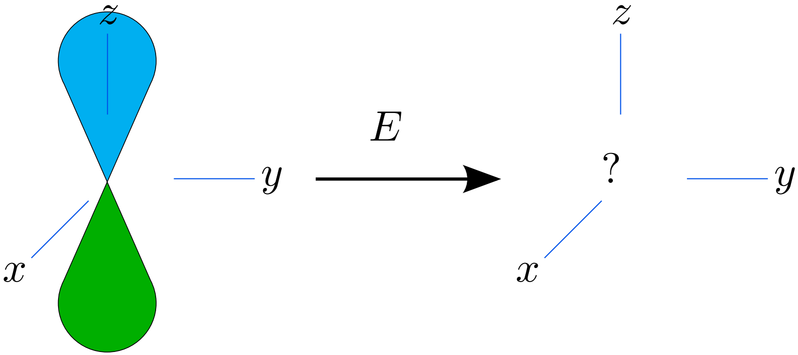
What happens when the E operation is applied?



- The E operation is a rotation by 360° about an arbitrary axis

Transformation Properties of a p_z Orbital in C_{2v}

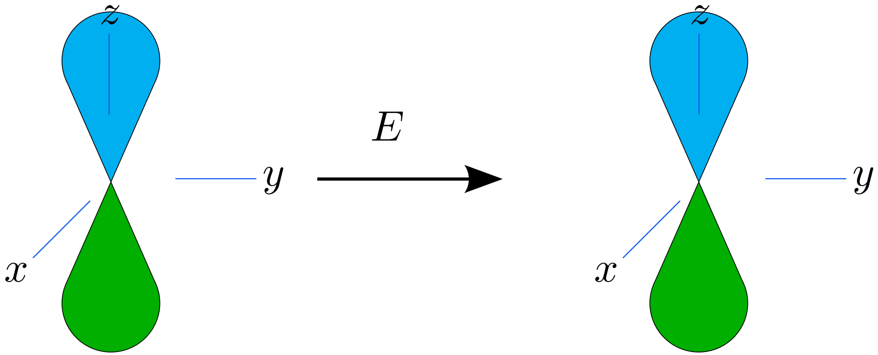
What happens when the E operation is applied?



- The E operation is a rotation by 360° about an arbitrary axis

Transformation Properties of a p_z Orbital in C_{2v}

The E operation returns the original configuration of the p_z orbital



- The result of this corresponds to a character of 1

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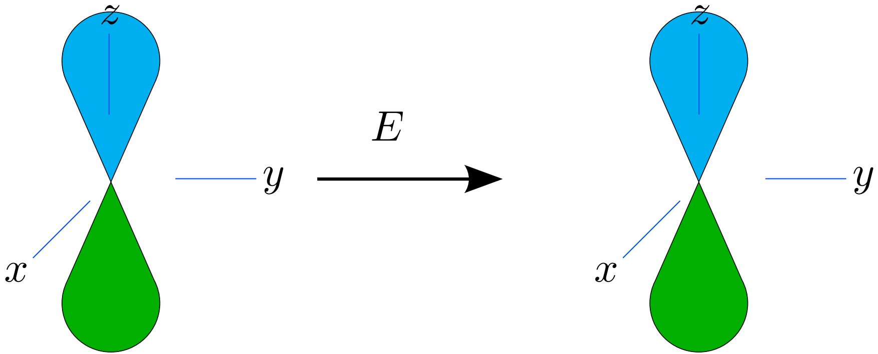

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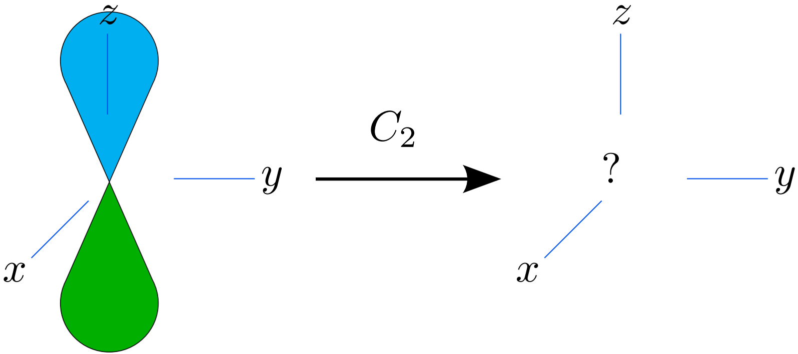
Transformation Properties of a p_z Orbital in C_{2v}

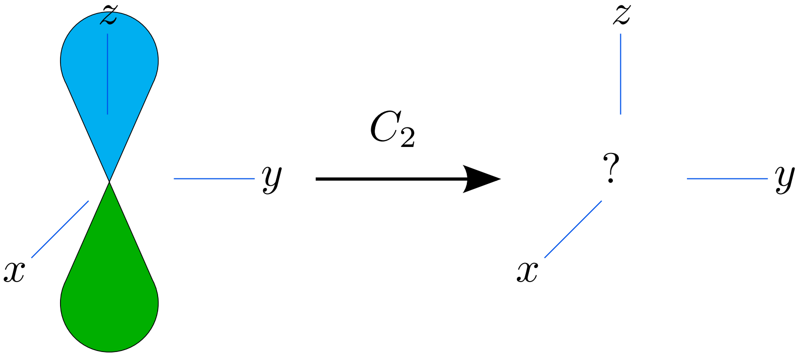
What happens when the C_2 operation is applied?



- The C_2 operation is a rotation by 180° about the z axis

Transformation Properties of a p_z Orbital in C_{2v}

What happens when the C_2 operation is applied?



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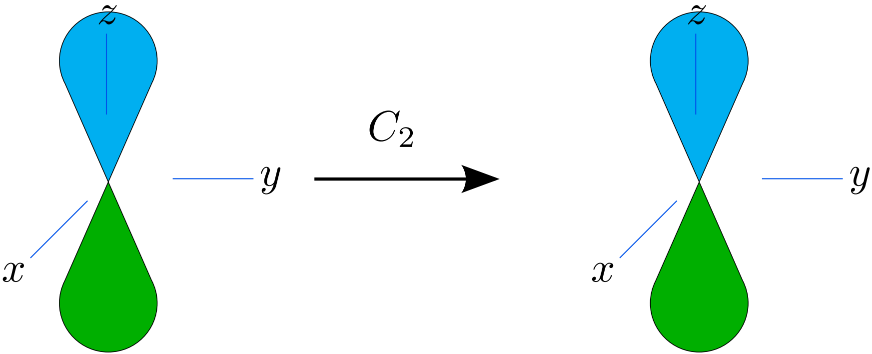
Transformation Properties of a p_z Orbital in C_{2v}

The C_2 operation does nothing to the phase of the p_z orbital



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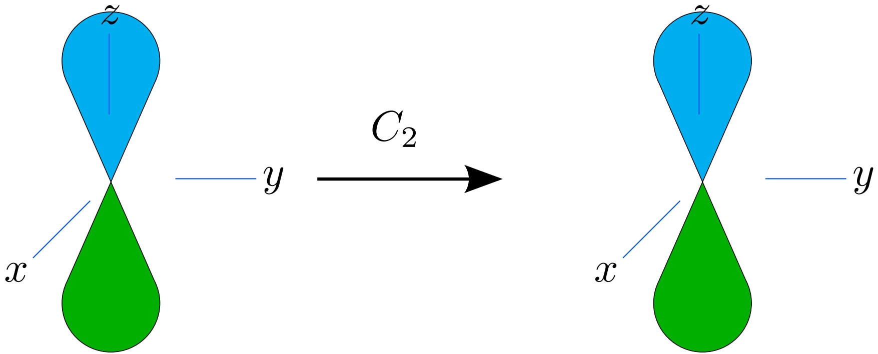

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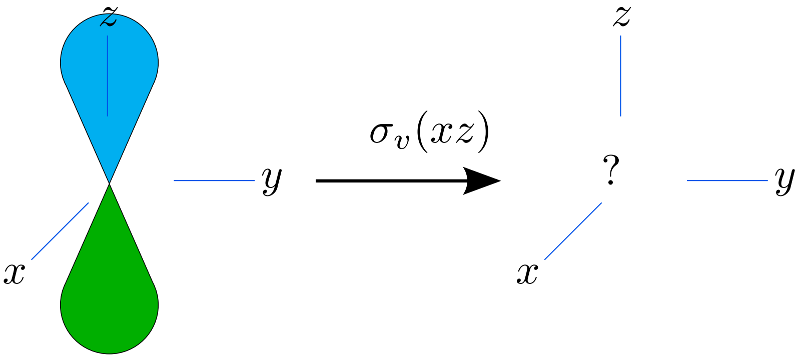
What happens when the $\sigma_v(xz)$ operation is applied?



- The $\sigma_v(xz)$ operation is a reflection through the xz plane

Transformation Properties of a p_z Orbital in C_{2v}

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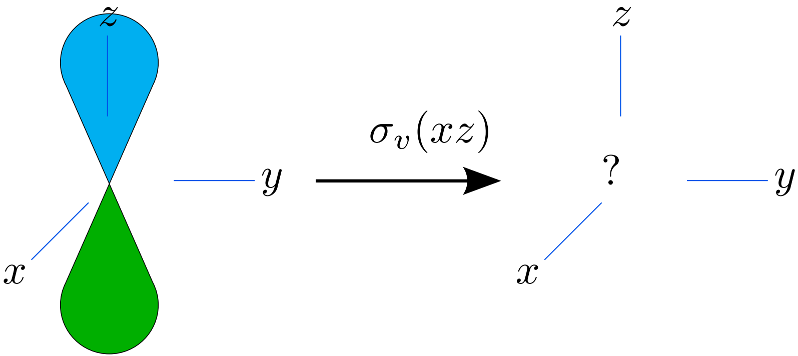

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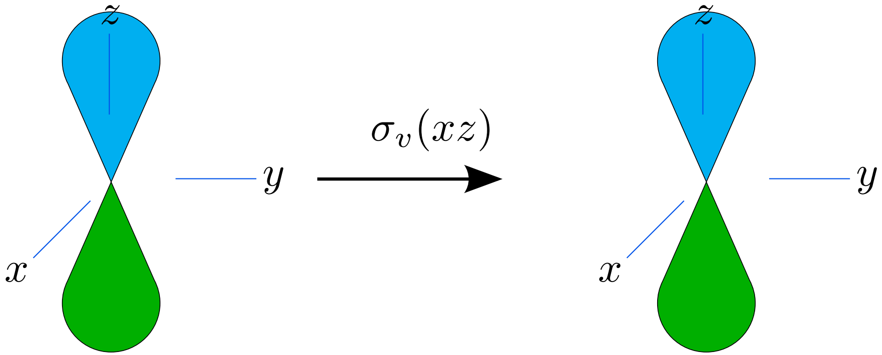
Transformation Properties of a p_z Orbital in C_{2v}

The $\sigma_v(xz)$ operation inverts the phase of the p_z orbital



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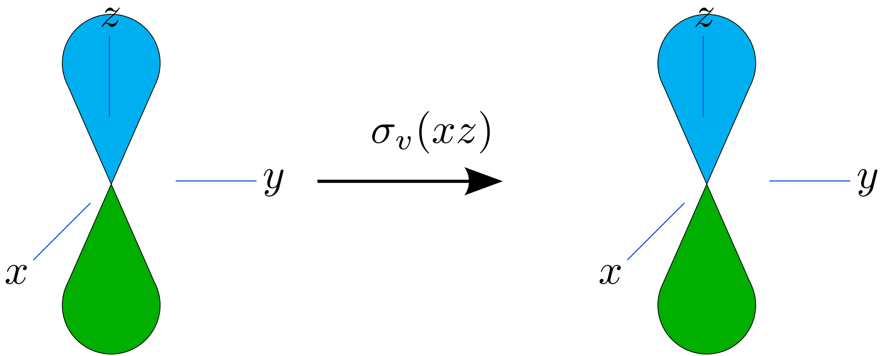

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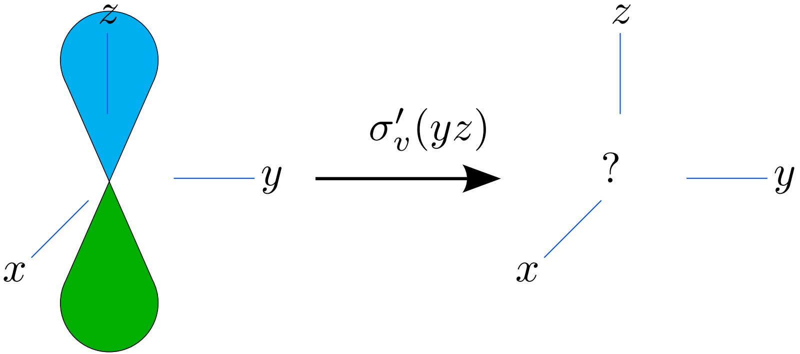
What happens when the $\sigma_v'(yz)$ operation is applied?



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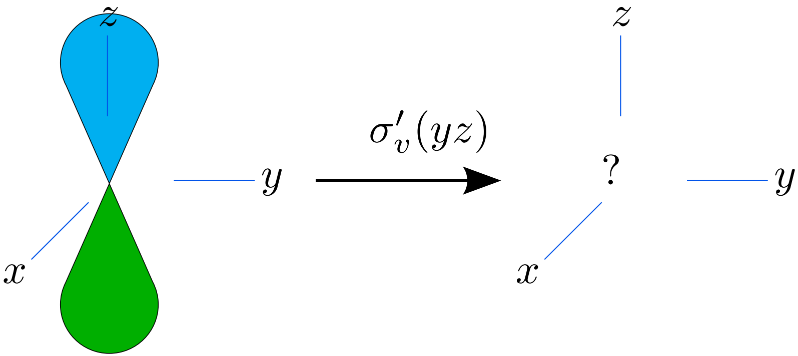

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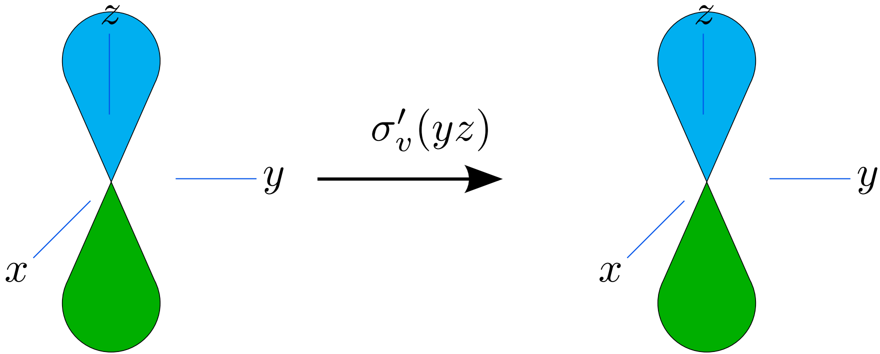

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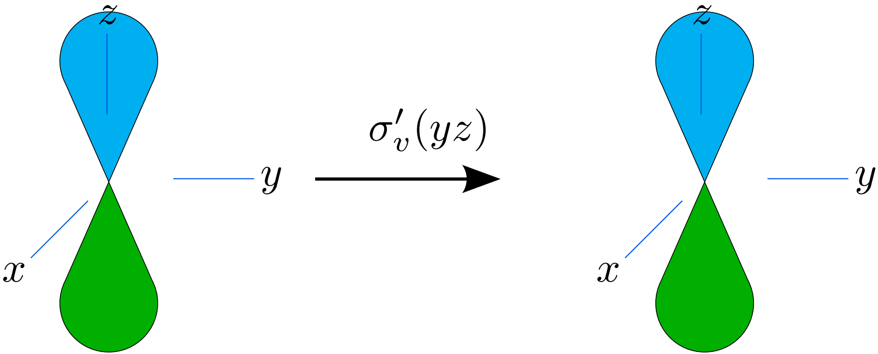

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Symmetry Restrictions on Molecular Orbitals (MOs)

- Only orbitals of the same symmetry may mix
- "Orbitals of the same symmetry" belong to the same irreducible representation
- For the C_{2v} water molecule, the oxygen s and p_z atomic orbitals may contribute to any molecular orbital of A_1 symmetry, but p_x and p_y may not
- Any valid molecular orbital must transform according to one of the irreducible representations of the molecular point group

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The C_{2v} Character Table

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v^{'}(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

The Molecular Orbitals of Water

- Notice that the water HOMO is a pure oxygen p_x orbital of B_1 symmetry
- The hydrogen atoms with their 1s valence orbitals lie in the nodal plane of the oxygen p_x orbital
- The two hydrogen 1s orbitals give rise to linear combinations of A_1 and B_2 symmetry
- The O-H bonding molecular orbitals must likewise be of A_1 and B_2 symmetry
- Given that all the irreducible representations of C_{2v} are singly degenerate, so must be all the MOs of the water molecule
- Click on Link to Water MOs

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