Symmetry Elements and Operations

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Outline

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A Molecule with Two Mirror Planes

The H_2O Molecule

- The O and H atoms lie in the same plane
- The plane of the molecule is a mirror plane, σ
- The plane $\perp$ to the molecular plane is a second σ
- The molecular plane is taken as the yz plane
- The mirrors are $\sigma_v(xz)$ and $\sigma'_v(yz)$
- The subscript v is for "vertical"

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Some Other Molecules

Does the molecule have a mirror plane?

- Ammonia, NH_3
- Sulfur tetrafluoride, SF_4
- Dioxygen, O_2
- White phosphorus, P_4
- Diborane, B_2H_6
- Myoglobin

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Molecules with Axes of Rotation, C_n

These have n-fold axes of rotation

What is n?

- Ammonia, NH_3
- Cubane, $(CH)_8$
- Water, H_2O
- Buckminsterfullerene, C_{60}
- Tick-Borne Encephalitis Virus

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Molecules with Axes of Rotation, C_n

Some observations based upon symmetry

- Ammonia, NH_3, has a single "higher-order" axis of rotation denoted C_3
- Molecules with a C_n axis where $n \geq 3$ have degenerate electronic energy levels
- Molecules with a C_n axis where $n \geq 3$ have degenerate vibrational energy levels
- Water, H_2O, has a single C_2 axis and thus has no degeneracies required by symmetry

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Molecules with Centers of Inversion

These have identical atoms with inverted coordinates

Is there an inversion center, *i*?

- Ethylene, C_2H_4
- Methane, CH_4
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Molecules with an Improper Axis of Rotation

A Combination of Rotation Axis and Mirror Plane

Consider $Pt(SH)_4{}^{2-}$

- Pt-S-H bonds are bent
- H atoms are located alternately above and below the PtS_4 plane
- There is not a C_4 axis
- There is not a mirror plane containing the four S atoms
- There is an S_4 axis passing through Pt and $\perp$ to sulfur plane

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The Identity Symmetry Element

This is present by default

- Rotation by 360° about an arbitrary axis returns an equivalent configuration
- This axis is referred to as the identity symmetry element, E

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Symmetry Operations

These are carried out with respect to symmetry elements

- A mirror plane, σ, generates a single reflection operation
- Two consecutive reflections with respect to a given σ is equivalent to the identity operation
- A C_2 axis generates a single two-fold rotation operation
- A C_3 axis generates two operations: rotation by $\frac{2\pi}{3}$ and rotation by $\frac{4\pi}{3}$
- The latter operations are called C_3 and C_3^2, respectively
- note that $C_3^3 = E$

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