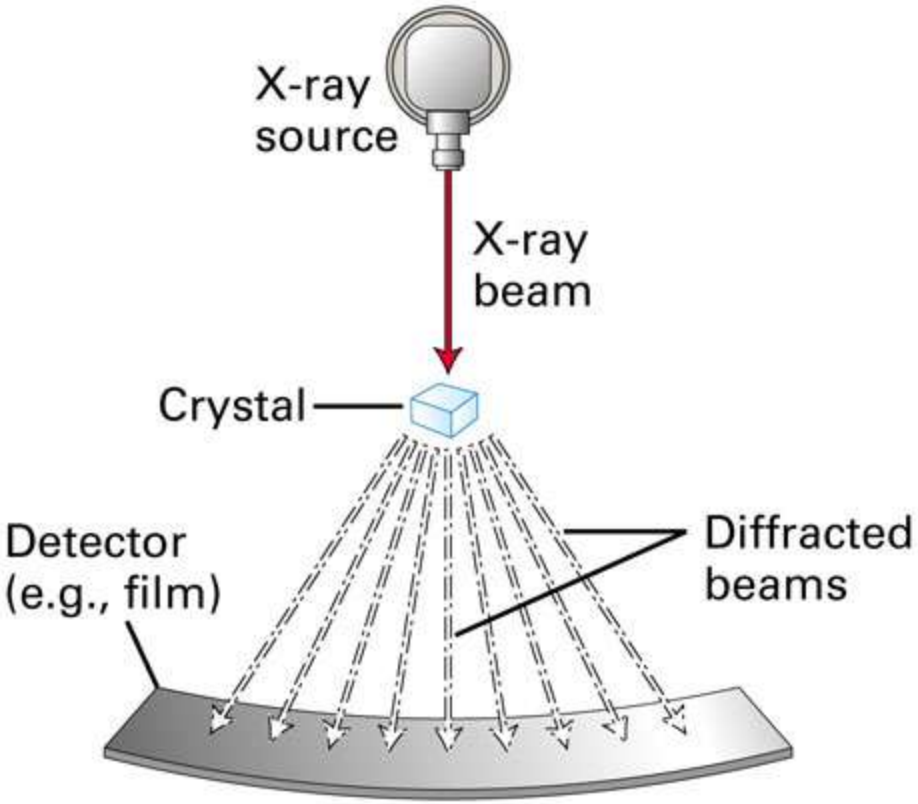
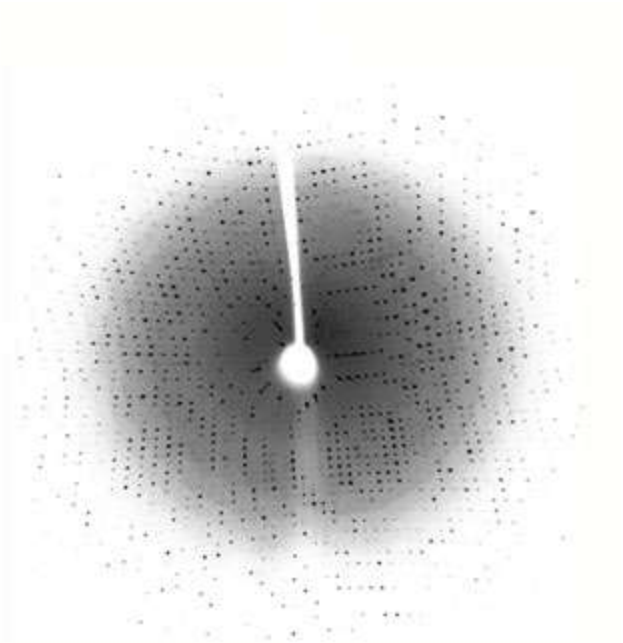
VSEPR THEORY AND MOLECULAR GEOMETRIES

VSEPR THEORY

- VSEPR (pronounced "vesper") stands for:
  - Valence Shell Electron Pair Repulsion
- It attempts to explain the 3-D shapes of molecules.
- How do we know what molecules look like?
  - X-Ray Crystallography
  - X-rays are fired through a crystallized sample of a substance and are diffracted in many directions.
  - By carefully studying the directions and intensity of the diffracted X-rays, a crystallographer can tell a lot about the locations of atoms within the crystal.
- Remember, theories explain observations!
  - VSEPR Theory explains the observed shapes of molecules.

X-RAY CRYSTALLOGRAPHY



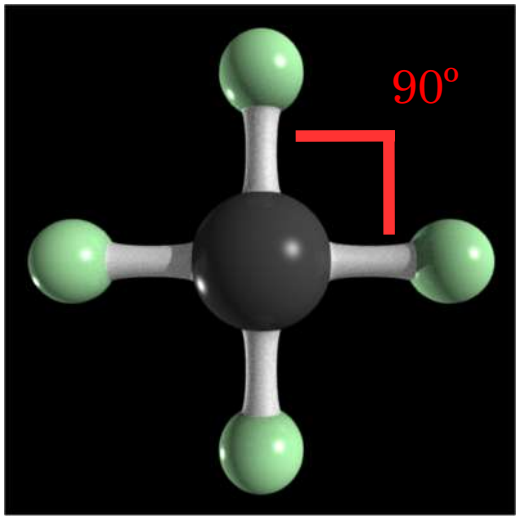


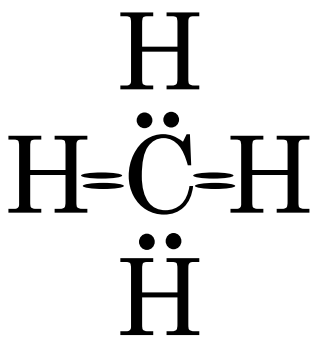
VSEPR THEORY

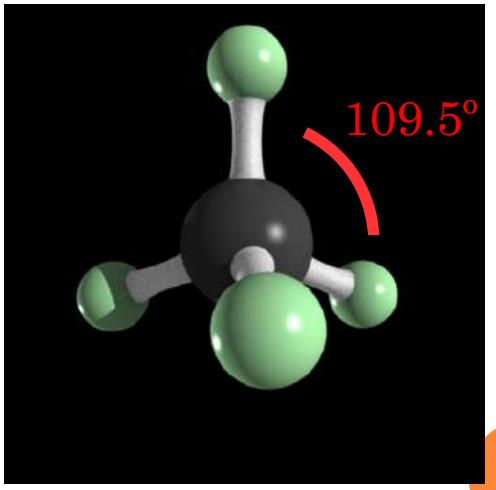
- The basic principles of VSEPR Theory:
  - Electron pairs repel each other.
  - Electron pairs in molecules tend to arrange themselves so as to minimize the repulsion between them.
    - In other words, get as far apart as possible.

THE GEOMETRY OF CH_4

- Based on the Lewis structure of methane, you might expect the geometry on the left.
  - VSEPR theory predicts the geometry on the right.
  - The geometry on the right is confirmed by observations.







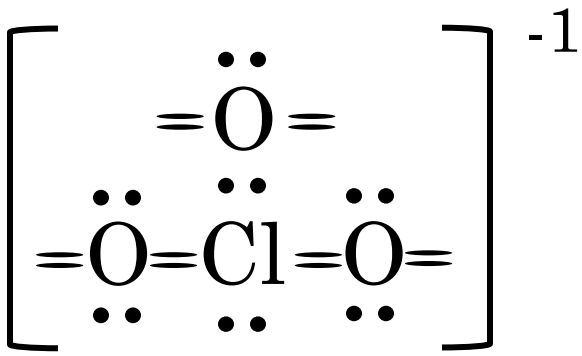
The spheres represent the centers of the carbon and hydrogen atoms.

VSEPR FORMULAS

- Lewis structures *do not* show geometry, only electron pair placement.
  - However, the 3-D shape (geometry) of a molecule *can* be determined from a properly-drawn Lewis structure.
- All monocentric molecules can be represented by a VSEPR formula:
- AXE
  - A = central atom
  - X = outer atoms (doesn't matter what they actually are or how many bonds they are held by)
  - E = lone pairs of electrons on the central atom only.

VSEPR FORMULAS

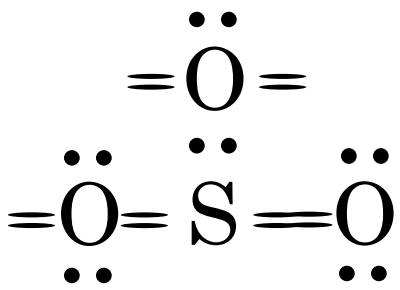
- What VSEPR formula corresponds to the chlorate ion, ClO_3^{-1}?
  - First draw a proper Lewis structure:
    - Needed = 32
    - Available = 26
    - Shared = 6



  - One central atom, three outer atoms, one lone pair:
    - AX_3E

VSEPR FORMULAS

- What VSEPR formula corresponds to sulfur trioxide, SO_3?
  - Draw a Lewis structure.
    - Needed = 32
    - Available = 24
    - Shared = 8



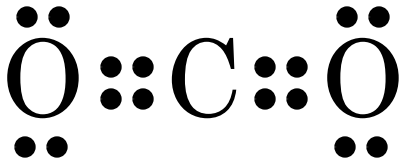
  - 1 central atom, 3 outer atoms, no lone pairs:
    - AX_3

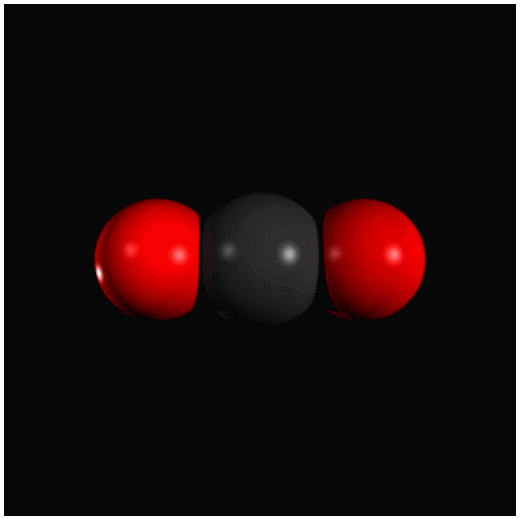
MOLECULAR GEOMETRIES

- Each VSEPR formula corresponds to a certain molecular geometry.
  - There are six possible geometries for molecules whose central atoms obey the octet rule.

MOLECULAR GEOMETRIES

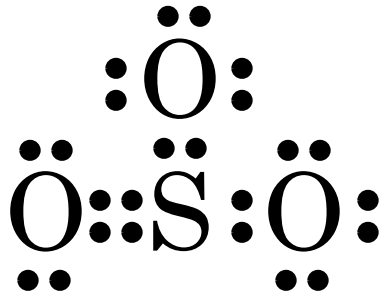
- VSEPR Formula: AX_2
- Geometry: Linear
- Bond Angle: 180°
- Example: CO_2

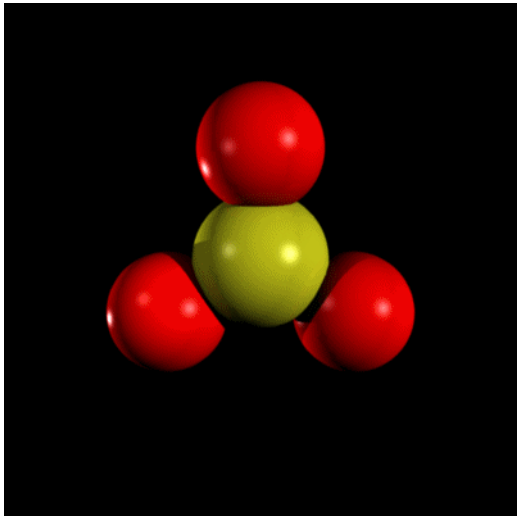




MOLECULAR GEOMETRIES

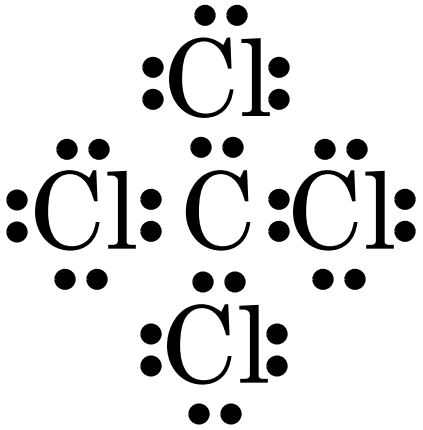
- VSEPR Formula: AX_3
- Geometry: Trigonal Planar
- Bond Angle: 120°
- Example: SO_3

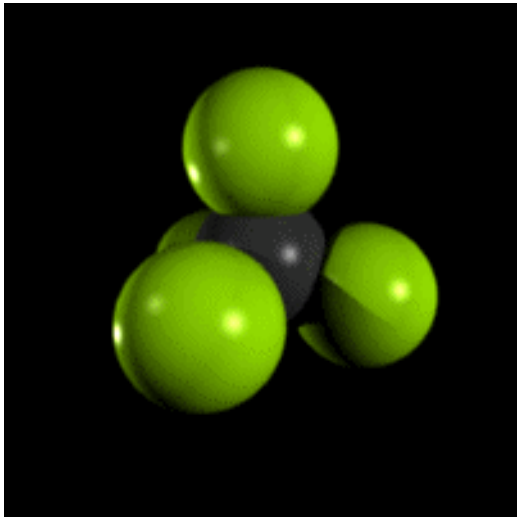




MOLECULAR GEOMETRIES

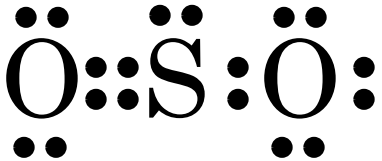
- VSEPR Formula: AX_4
- Geometry: Tetrahedral
- Bond Angle: 109.5°
- Example: CCl_4

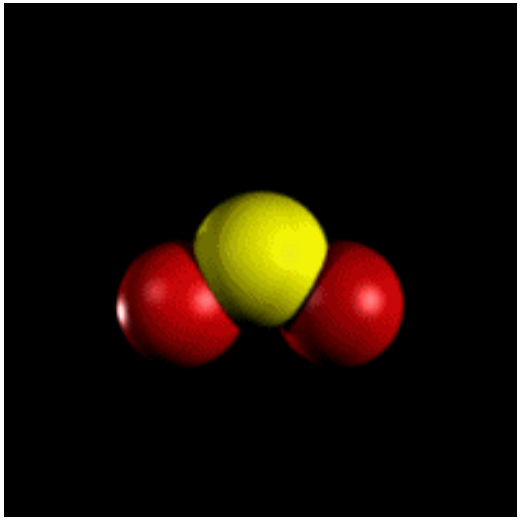




MOLECULAR GEOMETRIES

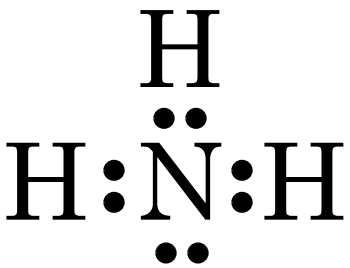
- VSEPR Formula: AX_2E
- Geometry: Bent (Angular)
- Bond Angle: Less than 120°
- Example: SO_2

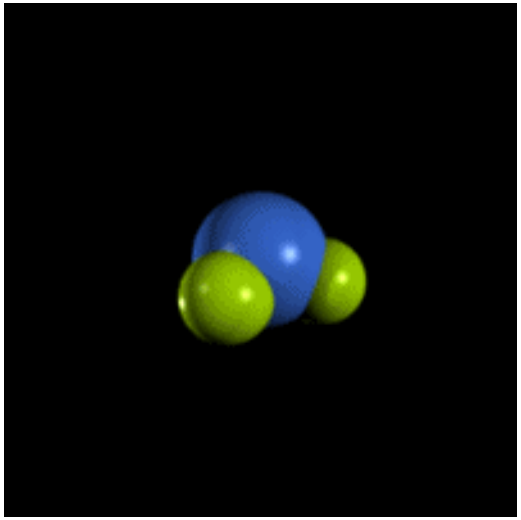




MOLECULAR GEOMETRIES

- VSEPR Formula: AX_3E
- Geometry: Trigonal Pyramidal
- Bond Angle: Less than 109.5°
- Example: NH_3





MOLECULAR GEOMETRIES

- VSEPR Formula: AX_2E_2
- Geometry: Bent (Angular)
- Bond Angle: Less than 109.5°
- Example: H_2O