VSEPR, Valence Shell Electron Pair Repulsion theory, allows one to predict molecular structure. If molecular structure can be predicted then molecular properties, like polarity, can be predicted.

The basic theory is that pairs of electrons repell each other; so, to minimize repulsion electron pairs try to be as far apart as possible.

1. First the number of electron pairs around the atoms must be counted.

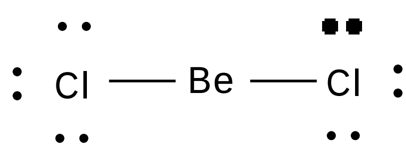
Multiple bonds are treated as though they are one pair, because the two bond must point in the same direction.

2. Then the pairs must be distributed in space to minimize pair replusions. Lone pairs take up more space than bonding pairs.

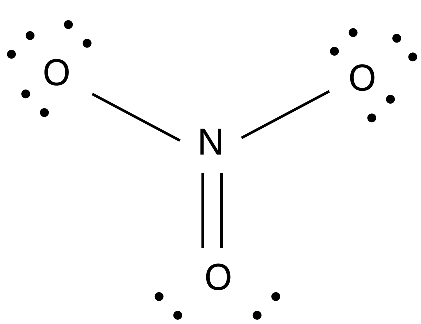
Numbers of pairs and the shapes the electrons form.

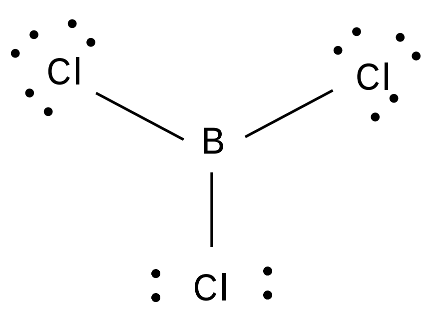
1 pair—linear H — H

2 pair—linear, electrons are 180° apart

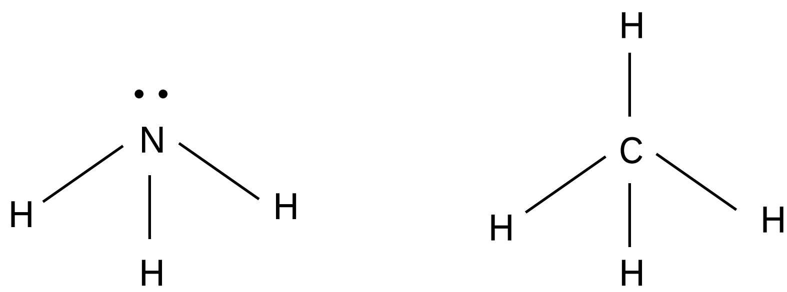


3 pair—trigonal planar, electrons are 120° apart

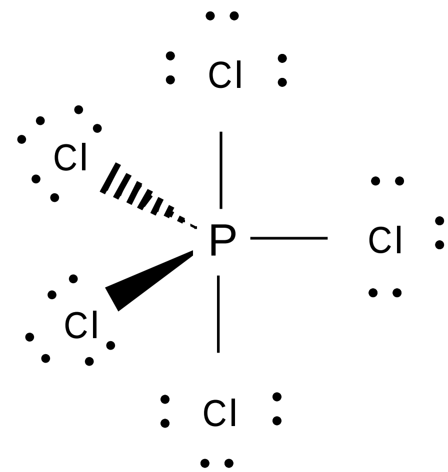




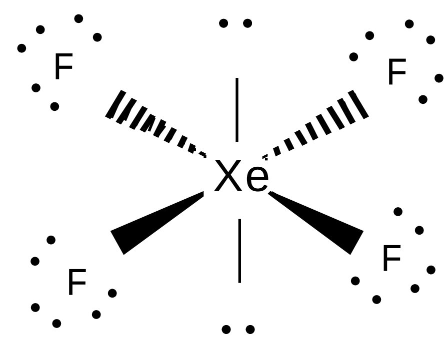
4 pair—tetrahedral, pairs are 109.5° apart



5 pair—trigonal bipyramid, triangular arrangement around the center, with a pair on top and bottom.



6 pair—octahedral, a pair of electrons along the positive and negative direction of each axis (x,y,z).



3. The positions of the atoms in the molecule are used to name the shape of the molecule

Shapes that can come from linear arrangement of electrons

Linear: Like CO_2 the bonds all line along one straight line.

Shapes that can come from trigonal planar arrangement of electrons

Bent: Three atoms in a non-linear arragement

Trigonal planar: (must be at least four atoms) one atom is at the center of the triangle, and the other three atoms are positioned on the vertices. Like SO_3, BCl_3, NO_3^-.

Shapes that can come from tetrahedral arrangement of electrons

Bent: Three atoms in a non-linear arragement, like H_2O.

Trigonal Pyramidal: (must be at least four atoms) one atom is at the center but is raised above the plane of the triangle, and the other three atoms are positioned on the vertices.

Tetrahedral: (must have at least five atoms) one atom is at the center of the tetrahedron, the other four atoms are positioned one at each vertex. Like CCl_4, CH_2Cl_2.

Shapes that can come from Trigonal Bipyramidal arrangement of electrons

Linear: Three atoms in a linear arrangement. Three empty verticies around the center occupied by lone pairs.

Bent: The bent arrangement is not likely. Three atoms in a non-linear arragement would mean that the three empty verticies occupied by lone pairs. Further, the lone pairs would be 90° degrees appart. It is more likely that a linear structure would result. Then the lone pairs are all 120° appart.

T-shaped: (must have four atoms) a central atom, one atom on the central triangle. One atom at the top and bottom verticies. The remaning triangle verticies iares occupied by lone pairs.

Trigonal planar: (must be at least four atoms) one atom is at the center of the triangle, and the other three atoms are positioned on the vertices. A pair of electrons occupies the top and bottom verticies. Tringonal planar is unlikely in that the lone pairs are 90° from bonding pairs. In the T-shape the lone pairs are 90° and 120° from other electron pairs. Of couse there is another possibility, but it too is unlikely.

See-Saw: (must have five atoms) 1 atom at the center, 2 around the trangle, and one at the top and bottom. The remaining vertex is occupied by a lone pair.

Trigonal Pyramidal: (must be at least five atoms) one atom is at the center but is raised above the plane of the triangle, and the other three atoms are positioned on the vertices. A lone pair occupies the final vertex. Trigonal pyramidal is unlikely because the lone pair is 90° from the three bonding pair, and if the structure adopted a see-saw geometry the lone pair is 90° and 120° from the bonding pairs.

Trigonal Bipyramidal: (must have at least 5 atoms) an atom at the center, triangular arrangement around the center, with an atom on top and bottom.

Common shapes that result from an Octahedral arrangement of electrons

Linear: Three atoms in a linear arrangement. Four empty verticies around the center are occupied by lone pairs.

T-shaped: (four atoms) a center atom and three other atoms arranged to form a T. This arrangement would be more stable than forming a pyramid with the atoms.

Square Planar: (must have at least 5 atoms) one atom at the center four others on the corners of the square. A piar of electrons occupies the top and bottom verticies. While a see-saw is possible, electron pair repulsions would be higher than the repulsions in the sqaure planar arrangment.

Square pyramidal: (must have atleast 6 atoms) one atom at the center of a square formed by four atoms, the sixth atom in a vertex directly above the center atom, and the bottom vertext occupied by a lone pair.

Octahedral: all six veticies, and the center position occupied by atoms.