

DIGONAL AND TRIGONAL COORDINATION OF VSEPR THEORY

Linear molecules

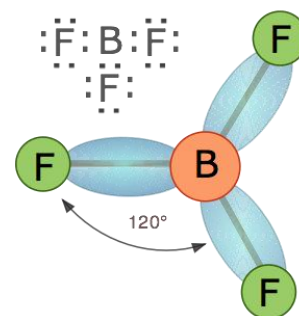
As we stated above, a simple triatomic molecule of the type AX₂ has its two bonding orbitals 180° apart, producing a molecule that we describe as having **linear** geometry.



Examples of triatomic molecules for which VSEPR theory predicts a linear shape are BeCl₂ (which, you will notice, doesn't possess enough electrons to conform to the octet rule) and CO₂. If you write out the electron dot formula for carbon dioxide, you will see that the C-O bonds are double bonds. This makes no difference to VSEPR theory; the central carbon atom is still joined to two other atoms, and the electron clouds that connect the two oxygen atoms are 180° apart.

Trigonal molecules

In an AX₃ molecule such as BF₃, there are three regions of electron density extending out from the central atom. The repulsion between these will be at a minimum when the angle between any two is $(360^\circ \div 3) = 120^\circ$. This requires that all four atoms be in the same plane; the resulting shape is called **trigonal planar**, or simply trigonal.



Summary of VSEPR theory

The VSEPR model is an extraordinarily powerful one, considering its great simplicity. Its application to predicting molecular structures can be summarized as follows:

1. Electron pairs surrounding a central atom repel each other; this repulsion will be minimized if the orbitals containing these electron pairs point as far away from each other as possible.
2. The coordination geometry around the central atom corresponds to the polyhedron whose number of vertices is equal to the number of surrounding electron pairs (coordination number). Except for the special case of 5, and the trivial cases of 2 and 3, the shape will be one of the regular polyhedra.

3. If some of the electron pairs are nonbonding, the shape of the molecule will be simpler than that of the coordination polyhedron.
4. Orbitals that contain nonbonding electrons are more concentrated near the central atom, and therefore offer more repulsion than bonding pairs to other orbitals.

While VSEPR theory is quite good at predicting the general shapes of most molecules, it cannot yield exact details. For example, it does not explain why the bond angle in H₂O is 104.5°, but that in H₂S is about 90°. This is not surprising, considering that the emphasis is on electronic repulsions, without regard to the detailed nature of the orbitals containing the electrons, and thus of the bonds themselves.