

Asity or probability envelopes lie closer to the oxygen nucleus) exert a greater mutual repulsion than the two bond pairs.^{[1]:410-417[11]}

A bond of higher bond order also exerts greater repulsion since the pi bond electrons contribute.^[11] For example in isobutylene, $(\text{H}_3\text{C})_2\text{C}=\text{CH}_2$, the $\text{H}_3\text{C}-\text{C}=\text{C}$ angle (124°) is larger than the $\text{H}_3\text{C}-\text{C}-\text{CH}_3$ angle (111.5°). However, in the carbonate ion, CO_3^{2-} , all three C-O bonds are equivalent with angles of 120° due to resonance.

AXE method

The "AXE method" of electron counting is commonly used when applying the VSEPR theory. The electron pairs around a central atom are represented by a formula AX_nE_m , where A represents the central atom and always has an implied subscript one. Each X represents a ligand (an atom bonded to A). Each E represents a lone pair of electrons on the central atom.^{[1]:410-417} The total number of X and E is known as the steric number. For example in a molecule AX_3E_2 , the atom A has a steric number of 5.

When the substituent (X) atoms are not all the same, the geometry is still approximately valid, but the bond angles may be slightly different from the ones where all the outside atoms are the same. For example, the double-bond carbons in alkenes like C_2H_4 are AX_3E_0 , but the bond angles are not all exactly 120° . Likewise, SOCl_2 is AX_3E_1 , but because the X substituents are not identical, the X-A-X angles are not all equal.

Based on the steric number and distribution of Xs and Es, VSEPR theory makes the predictions in the following tables.

Main-group elements

For main-group elements, there are stereochemically active lone pairs E whose number can vary between 0 to 3. Note that the geometries are named according to the atomic positions only and not the electron arrangement. For example, the description of AX_2E_1 as a bent molecule means that the three atoms AX_2 are not in one straight line, although the lone pairs help to determine the geometry.