Shapes of simple molecules and ions

VSEPR THEORY

The shapes of simple molecules and ions can be determined by using the valence shell electron pair repulsion (VSEPR) theory. This states that pairs of electrons arrange themselves around the central atom so that they are as far apart from each other as possible. There will be greater repulsion between non-bonded pairs of electrons than between bonded pairs. Since all the electrons in a multiple bond must lie in the same direction, double and triple bonds count as one pair of electrons. Strictly speaking the theory refers to negative charge centres, but for most molecules this equates to pairs of electrons.

This results in five basic shapes depending on the number of pairs.

No. of charge centres	Shape	Name of shape	Bond angle(s)
2	0-0-0	linear	180°
3	0	trigonal planar	120°
4	0	tetrahedral	109.5°
5	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	trigonal bipyramidal	90°, 120°, 180°
6	0-0-0	octahedral	90°, 180°
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WORKING OUT THE ACTUAL SHAPE

To work out the actual shape of a molecule calculate the number of pairs of electrons around the *central* atom, then work out how many are bonding pairs and how many are non-bonding pairs. (For ions the number of electrons which equate to the charge on the ion must also be included when calculating the total number of electrons.)

2 NEGATIVE CHARGE CENTRES

CI-Be-CI O=C=O $H-C\equiv C-H$ $H-C\equiv N$ double bond triple bond counts as one pair counts as one pair

3 NEGATIVE CHARGE CENTRES

3 bonding pairs - trigonal planar

$$B = H C = C$$

2 bonding pairs, 1 non-bonded pair - bent or V-shaped



nitrite ion

5 AND 6 NEGATIVE CHARGE CENTRES

5 and 6 negative charge centres

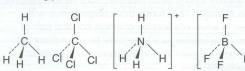
octahedral square planar non-bonding pairs as far apart as possible above and below plane



distorted tetrahedral

4 NEGATIVE CHARGE CENTRES

4 bonding pairs - tetrahedral



ammonium ion tetrafluoroborate

3 bonding pairs, 1 non-bonding pair - trigonal pyramid



greater repulsion by non-bonding pair .. bond angle smaller than 109.5°

2 bonding pairs, 2 non-bonding pairs - bent or V-shaped

even greater repulsion by two non-bonding pairs so bond angle even smaller

trigonal

bipyramidal