1.5: Valence-Shell Electron-Pair Repulsion Theory (VSEPR)

The **Valence-Shell Electron-Pair Repulsion (VSEPR)** theory helps us to understand and predict the geometry (shape) of molecules or ions. The theory is:

- Electron pairs repel each other whether they are in chemical bonds or lone pairs.
- Valence electron pairs are oriented to be as far apart as possible to minimize repulsions.

Based on this theory, depending on the number of electron pairs (both bonding pairs and lone pairs) around the central atom, a certain shape is adopted to minimize the repulsion between election pairs, as summarized in the table below:

Total number of electron groups (electron pairs) around central atom	Geometry (Shape) of electron groups (electron pairs)
2	linear
3	trigonal planar
4	tetrahedral
5	trigonal bipyramidal
6	octahedral

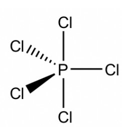
Table 1.1 Basic VSEPR Shapes

Notes:

- For VSEPR purpose, the terms "**shape**" and "**geometry**" are interchangeable; "**electron pair**" and "**electron group**" are also interchangeable.
- Multiple bonds (double or triple bond) are regarded as **one electron group** for VSEPR purpose.

For species that do not have any lone pair electrons (LP), the geometry (shape) of the species is just the same as the geometry of the electron groups.

For the exampleof the PCl_5molecule, there are five electron groups on the central phosphorous, and they are all bonding pairs (BP). The shape of the electron groups is trigonal bipyramidal, and the shape of the PCl_5 molecule is trigonal bipyramidal as well. The trigonal bipyramidal shape can be drawn on paper using solid and dashed wedges: the three bonds lie within the paper plane are shown as ordinary lines, the solid wedge represent a bond that points out of the paper plane, and the dashed wedge represent a bond that points behind the paper plane.



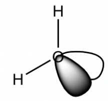
trigonal bipyramidal shape of PCl_5 molecule

Figure1.5a Tigonal bipyramidal shape of PCl5 molecule

However, for the species that has lone pair electrons on the central atom, the shape of the species will be *different* to the shape of the electron groups. The reason is that even though the lone pairs occupy the space, there are no terminal atoms connected with lone pair, so the lone pair become "invisible" for the shape of the species.

For the example of the water (H_2O) molecule, the central oxygen atom has two BPs and two LPs, and the shape of all the electron groups is tetrahedral. The shape of a water molecule is bent because only the atoms are counted towards the molecular shape, not the lone pair electrons.

https://chem.libretexts.org/@go/page/359565



bent shape of H_2O molecule

Figure 1.5b Bent shape of H20 molecule

The VSEPR shapes can be rather diverse, considering the different numbers of total electron pairs together with the different numbers of lone pairs involved. The most common shapes are summarized in the following table (Table 1.2). To describe a certain shape, the specific name has to be used properly, and the bond angle information is important as well.

Total number of e-groups	Geometry (shape) of**all** the **electron groups**	# of Bonding Pairs (BP) and Lone Pairs (LP)	Geometry (shape) of the **species**	Angles (°)
2	linear	2BP	linear	180
3	trigonal planar	3BP	trigonal planar	120
		2BP, 1LP	bent	<120
4	tetrahedral	4BP	tetrahedral	109.5
		3BP, 1LP	trigonal pyramidal	<109.5
		2BP, 2LP	bent	<109.5
5	trigonal bipyramidal	5BP	trigonal bipyramidal	120, 90, 180
		4BP, 1LP	see-saw	<120, 90, 180
		3BP, 2LP	T-shape	90, 180
		2BP, 3LP	linear	180
6	octahedral	6BP	octahedral	90, 180
		5BP, 1LP	square pyramidal	90, 180
		4BP, 2LP	square planar	90, 180

Table 1.2 Summary of specific VSEPR shapes

The website **https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html** provides good resources for visualizing and practicing VSEPR topics.

We will see more applications of VSEPR in organic compounds in next section.

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